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UTILITY PATENT APPLICATION TRANSMITTAL

(Only for new nonprovisional applications under 37 C.F.R. § 1.53(b))

Attorney Docket No.	2459-1-003
First Inventor or Application Identifier	Ming-Ming Zhou
Title	METHODS OF IDENTIFYING ...
Express Mail Label No.	EL485954545US

02/22/00 jc682 U.S. PTO

02/22/00 jc525 U.S. PTO 09/510114

APPLICATION ELEMENTS

See MPEP chapter 600 concerning utility patent application contents.

ADDRESS TO: Assistant Commissioner for Patents
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1. [ ] * Fee Transmittal Form *(e.g., PTO/SB/17)*
(Submit an original and a duplicate for fee processing)
2. [✓] Specification [Total Pages 67]
(preferred arrangement set forth below)
- Descriptive title of the Invention
- Cross References to Related Applications
- Statement Regarding Fed sponsored R & D
- Reference to Microfiche Appendix
- Background of the Invention
- Brief Summary of the Invention
- Brief Description of the Drawings *(if filed)*
- Detailed Description
- Claim(s)
- Abstract of the Disclosure
3. [✓] Drawing(s) *(35 U.S.C. 113)* [Total Sheets 9]
4. Oath or Declaration unexecuted [Total Pages 3]
   a. [ ] Newly executed (original or copy)
   b. [ ] Copy from a prior application (37 C.F.R. § 1.63(d))
   (for continuation/divisional with Box 16 completed)
      i. [ ] DELETION OF INVENTOR(S)
      Signed statement attached deleting inventor(s) named in the prior application, see 37 C.F.R. §§ 1.63(d)(2) and 1.33(b).

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5. [ ] Microfiche Computer Program *(Appendix)*
6. Nucleotide and/or Amino Acid Sequence Submission
(if applicable, all necessary)
   a. [✓] Computer Readable Copy
   b. [✓] Paper Copy (identical to computer copy)
   c. [✓] Statement verifying identity of above copies

ACCOMPANYING APPLICATION PARTS

7. [ ] Assignment Papers (cover sheet & document(s))
8. [ ] 37 C.F.R.§3.73(b) Statement *(when there is an assignee)* [ ] Power of Attorney
9. [ ] English Translation Document *(if applicable)*
10. [ ] Information Disclosure Statement (IDS)/PTO-1449 [ ] Copies of IDS Citations
11. [ ] Preliminary Amendment
12. [✓] Return Receipt Postcard (MPEP 503)
(Should be specifically itemized)
13. [ ] * Small Entity Statement(s) *(PTO/SB/09-12)* [ ] Statement filed in prior application, Status still proper and desired
14. [ ] Certified Copy of Priority Document(s)
(if foreign priority is claimed)
15. [X] Other: atomic coordinates in 6 Tables

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[ ] Continuation [ ] Divisional [ ] Continuation-in-part (CIP) of prior application No: _____

Prior application information: Examiner _____ *Group / Art Unit:* _____

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METHODS OF IDENTIFYING MODULATORS OF BROMODOMAINS

FIELD OF THE INVENTION

The present invention provides the three-dimensional structure of a histone acetyltransferase bromodomain. The three-dimensional structural information is included in the invention. The present invention also identifies for the first time, that bromodomains can bind to an acetylated binding partners. The interaction between bromodomains and their binding partners play a crucial role in various cellular functions, including in the regulation/modulation of DNA transcription. Therefore, the present invention provides procedures for identifying agents that can modulate the interaction of bromodomains and their binding partners by high throughput drug screening and/or through the use of rational drug design based on the three-dimensional data provided herein.

BACKGROUND OF THE INVENTION

In recent years great strides have been made in the elucidation of the steps involved in intercellular and intracellular signaling. Indeed, the individual steps of the cascade of events involved in a number of cellular signal transduction processes have been determined. For example, intercellular signal transduction generally begins with an intercellular ligand binding the extracellular portion of a receptor of the plasma membrane. The bound receptor then either directly or indirectly initiates the activation of one or more cellular factors. An activated cellular factor may act as transcription factor by entering the nucleus to interact with its corresponding genomic response element, or alternatively, it may interact with other cellular factors depending on the complexity of the process. In either case, one or more transcription factors ultimately bind to one or more specific genomic response elements. This binding plays a crucial role in the up and/or down regulation of the transcription of the specific genes that are under the control of these genomic response elements. However, the process of re-organizing the chromatin of eukaryotic cells, which is a prerequisite for the binding of the transcription factor to the genomic response elements, has remained a mystery.

Chromatin contains several highly conserved histone proteins including: H3, H4, H2A, H2B, and H1. These histone proteins package eukaryotic DNA into repeating nucleosomal units that are folded into higher-order chromatin fibers [Luger and Richmond, *Curr. Opin. Genet. Dev.* **8:**140-146 (1998)]. A portion of the histone that comprises roughly a quarter of the protein protrudes from the chromatin surface, and is thereby sensitive to proteolytic enzymes [van Holde, in *Chromatin* (Rich, A,. *ed.*, Springer, New York) pages111-148 (1988); Hect *et al.*, *Cell* **80**:583-592 (1995)]. This portion of the histone is known as the "histone tail". Histone tails tend to be free for protein-protein interaction, and are also the portion of the histone most prone to post-translational modification. Such post-translational modification includes acetylation, phosphorylation, methylation, ubiquitination, and ADP-ribosylation [van Holde, in *Chromatin* (Rich, A,. *ed.*, Springer, New York) pages111-148 (1988)].

Of all classes of proteins, histones are amongst the most susceptible to post-translational modification. Perhaps the best studied post-translational modification of histones is the acetylation of specific lysine residues [Grunstin, M., *Nature*, **389:**349-352 (1997)]. Indeed, acetylation of histone lysine residues has been suggested to play a pivotal role in chromatin remodeling and gene activation. Consistently, distinct classes of enzymes, namely histone acetyltransferases (HATs) and histone deacetylases (HDACs), acetylate or de-acetylate specific histone lysine residues [Struhl, *Genes Dev.* **12**:599-606 (1998)].

Nearly all known nuclear HATs contain an approximately 110 amino acid sequence known as the bromodomain [Jeanmougin *et al.*, Trends in Biochemical *Sciences*, **22:**151-153 (1997)], a protein motif that was initially discovered in Drosophila brahma protein. Bromodomains are found in a large number of chromatin-associated proteins and have now been identified in approximately 40 proteins, often adjacent to other protein motifs [Jeanmougin *et al.*, *Trends in Biochemical Sciences*, **22:**151-153 (1997); Tamkun *et al.*, *Cell*, **68:**561-572 (1992): Hanes *et al.*, *Nucleic Acids Research*, **20:**2603 (1992)]. Proteins that contain a bromodomain often contain a second bromodomain. However, despite the wide occurrence of bromodomains and their

likely role in chromatin regulation, their three-dimensional structure and binding partners heretofore have remained unknown.

Therefore, there is a need to identify a binding partner for a bromodomain. In addition, there is a need to identify agonists or antagonists to the bromodomain-binding partner complex. Since a preferred method of drug-screening relies on structure based drug design, there is also a need to determine the three-dimensional structure of a bromodomain. In this case, once the three dimensional structure of bromodomain is determined, potential agonists and/or potential antagonists can be designed with the aid of computer modeling [Bugg *et al.*, *Scientific American*, **Dec.**:92-98 (1993); West *et al.*, *TIPS*, **16**:67-74 (1995); Dunbrack *et al.*, *Folding & Design,* **2**:27-42 (1997)]. However, heretofore the three-dimensional structure of the bromodomain has remained unknown. Therefore, there is a need for obtaining a form of the bromodomain that is amenable for NMR analysis and/or X-ray crystallographic analysis. Furthermore, there is a need for the determination of the three-dimensional structure of the bromodomain. Finally, there is a need for procedures for related structural based drug design predicated on such structural data.

The citation of any reference herein should not be construed as an admission that such reference is available as "Prior Art" to the instant application.

SUMMARY OF THE INVENTION

The present invention provides, for the first time, that bromodomains bind to acetyl-lysine residues of proteins. The present invention also provides the three-dimensional structure of a bromodomain as well as the three-dimensional structure of a bromodomain-acetyl-histamine complex. The structural information provided can be employed in methods of identifying drugs that can modulate the cellular processes that involve bromodomain-acetyl-lysine interactions. These interactions include chromatin remodeling, which is a required step in eukaryotic transcription. In a particular embodiment, the three-dimensional structural information is used in the design of an inhibitor of leukemia.

The present invention provides an isolated nucleic acid that encodes a peptide consisting of about 21 to 40 amino acids that comprises a ZA loop of a bromodomain. In a preferred embodiment the peptide comprises about 23 to 34 amino acids. The isolated nucleic acid can further comprise a heterologous nucleotide sequence.

In a preferred embodiment the peptide comprises the amino acid sequence of SEQ ID NO:3. In another embodiment the peptide comprises the amino acid sequence of SEQ ID NO:43. In particular embodiments the ZA loop is obtained from the bromodomain having the amino acid sequence of SEQ ID NO:7, or SEQ ID NO:8, or SEQ ID NO:9, or SEQ ID NO:10, or SEQ ID NO:11, or SEQ ID NO:12, or SEQ ID NO:13, or SEQ ID NO:14, or SEQ ID NO:15, or SEQ ID NO:16, or SEQ ID NO:17, or SEQ ID NO:18, or SEQ ID NO:19, or SEQ ID NO:20, or SEQ ID NO:21,or SEQ ID NO: 22, or SEQ ID NO:23, or SEQ ID NO:24, or SEQ ID NO:25, or SEQ ID NO:26, or SEQ ID NO:27, or SEQ ID NO:28, or SEQ ID NO:29, or SEQ ID NO:30, or SEQ ID NO: or SEQ ID NO:31, or SEQ ID NO:32,or SEQ ID NO: 33, or SEQ ID NO:34, or SEQ ID NO:35, or SEQ ID NO:36 , or SEQ ID NO:37, or SEQ ID NO:38, or SEQ ID NO: or SEQ ID NO:39, or SEQ ID NO:40, or SEQ ID NO:41, or SEQ ID NO:42.

The present invention further provides a recombinant DNA molecule that comprises an isolated nucleic acid of the present invention, as described above, with or without a heterologous nucleotide sequence. Such a recombinant DNA molecule can be operatively linked to an expression control sequence and can be part of an expression vector. The present invention further provides a cell that comprises such an expression vector. The cell can be either a eukaryotic or a prokaryotic cell. The present invention further provides a method of expressing the peptides of the present invention or fragments thereof in this cell. One such method comprises culturing the cell in an appropriate cell culture medium under conditions that provide for expression of the peptide by the cell.

The present invention further provides a peptide consisting of about 21 to 40 amino acids that comprises a ZA loop of a bromodomain. In a preferred embodiment the

peptide comprises about 23 to 34 amino acids. The present invention also provides fusion proteins or peptides comprising these peptides.

In a preferred embodiment the peptide comprises the amino acid sequence of SEQ ID NO:3. In another embodiment the peptide comprises the amino acid sequence of SEQ ID NO:43. In particular embodiments the ZA loop is obtained from the bromodomain having the amino acid sequence of SEQ ID NO:7, or SEQ ID NO:8, or SEQ ID NO:9, or SEQ ID NO:10, or SEQ ID NO:11, or SEQ ID NO:12, or SEQ ID NO:13, or SEQ ID NO:14, or SEQ ID NO:15, or SEQ ID NO:16, or SEQ ID NO:17, or SEQ ID NO:18, or SEQ ID NO:19, or SEQ ID NO:20, or SEQ ID NO:21,or SEQ ID NO: 22, or SEQ ID NO:23, or SEQ ID NO:24, or SEQ ID NO:25, or SEQ ID NO:26, or SEQ ID NO:27, or SEQ ID NO:28, or SEQ ID NO:29, or SEQ ID NO:30, or SEQ ID NO: or SEQ ID NO:31, or SEQ ID NO:32,or SEQ ID NO: 33, or SEQ ID NO:34, or SEQ ID NO:35, or SEQ ID NO:36 , or SEQ ID NO:37, or SEQ ID NO:38, or SEQ ID NO: or SEQ ID NO:39, or SEQ ID NO:40, or SEQ ID NO:41, or SEQ ID NO:42.

The present invention also provides antibodies raised against the peptides/proteins of the present invention, or raised against an antigenic fragment of these proteins/fragments. In a particular embodiment an antibody is raised against a fragment of the ZA loop of a bromodomain. In another embodiment an antibody is raised against a fragment of a protein or peptide that comprises an acetyl-lysine, wherein the protein or peptide can bind to a bromodomain. Such fragments can be conjugated to a carrier protein or be part of a fusion protein. In one embodiment the antibody is a polyclonal antibody. In another embodiment, the antibody is a monoclonal antibody. A hybridoma that makes the monoclonal antibody is also part of the present invention. In a particular embodiment the antibody is a chimeric antibody. Antibodies that can specifically recognize acetyl-lysine residues involved bromodomain binding are also part of the present invention.

In another aspect of the present invention a method is provided for identifying a compound that modulates the affinity of a bromodomain for a ligand (and/or protein) that comprises an acetylated lysine. One such embodiment comprises contacting the

bromodomain and the ligand in the presence of a compound under conditions that , the bromodomain and the ligand bind in the absence of the compound. The affinity of the bromodomain for the ligand is then determined (*e.g.*, measured). A compound is identified as a compound that modulates the affinty of the bromodomain for the ligand when there is a change in the affinity of the bromodomain for the ligand in the presence of the compound. When the affinity of the bromodomain for the ligand increases in the presence of the compound, the compound is identified as a promoting agent for the bromodomain-ligand complex. When the affinity of the bromodomain for the ligand decreases in the presence of the compound, the compound is identified as an inhibitor of the bromodomain-ligand complex. In a preferred embodiment, the compound to be tested is pre-selected by performing rational drug design with the set of atomic coordinates obtained from one or more of Tables 1-6. More preferably the selecting is performed in conjunction with computer modeling. In a particular embodiment, the compound is selected by performing rational drug design with the set of atomic coordinates obtained from a set of atomic coordinates defining the three-dimensional structure of a bromodomain consisting of the amino acid sequence of SEQ ID NO:7 alone or with acetyl-histamine.

The present invention also provides a method of identifying a compound that modulates the stability of a bromodomain-acetyl-lysine binding complex. One such embodiment comprises contacting the bromodomain-acetyl-lysine binding complex in the presence of the compound under conditions in which the bromodomain-acetyl-lysine binding complex forms in the absence of the compound. The stability of the bromodomain-acetyl-lysine binding complex is then determined (*e.g.*, measured). A compound is identified as a compound that modulates the stability of the bromodomain-acetyl-lysine binding complex, when there is a change in the stability of the bromodomain-acetyl-lysine binding complex in the presence of that compound. When the stability of the bromodomain-acetyl-lysine binding complex increases in the presence of the compound, the compound is identified as a stabilizing agent. When the stability of the bromodomain-acetyl-lysine binding complex decreases in the presence of the compound, the compound is identified as an inhibitor. In a preferred embodiment, the compound to be tested is pre-selected by performing rational drug

design with the set of atomic coordinates obtained from one or more of Tables 1-6. More preferably the selecting is performed in conjunction with computer modeling. In a particular embodiment, the compound is selected by performing rational drug design with the set of atomic coordinates obtained from a set of atomic coordinates defining the three-dimensional structure of a bromodomain consisting of the amino acid sequence of SEQ ID NO:7 alone or with acetyl-histamine.

As anyone having skill in the art of drug development would readily understand, the potential drugs selected by the above methodologies can be refined by re-testing in appropriate drug assays, including those disclosed herein. Chemical analogs of such potential drugs can be obtained (either through chemical synthesis or drug libraries) and be analogously tested. Therefore, methods comprising successive iterations of the steps of the individual drug assays, as exemplified herein, using either repetitive or different binding studies, or transcription activation studies or other such studies are envisioned in the present invention. In addition, potential drugs may be identified first by rapid throughput drug screening, as described below, prior to performing computer modeling on a potential drug using the three-dimensional structure of the bromodomain.

The present invention further comprises all of the potential, selected, and putative compounds (drugs) identified by the methods of the present invention, as well as the final drugs themselves identified with the methods of the present invention.

The present invention further provides a method for identifying a potential binding partner for a protein (*e.g.*, a histone) comprising an acetyl-lysine. One such embodiment comprises contacting the protein with a polypeptide comprising a bromodomain. In a preferred embodiment the bromodomain comprises the amino acid sequence of SEQ ID NO:3. In particular embodiments the bromodomain has the amino acid sequence of SEQ ID NO:7, or SEQ ID NO:8, or SEQ ID NO:9, or SEQ ID NO:10, or SEQ ID NO:11, or SEQ ID NO:12, or SEQ ID NO:13, or SEQ ID NO:14, or SEQ ID NO:15, or SEQ ID NO:16, or SEQ ID NO:17, or SEQ ID NO:18, or SEQ ID NO:19, or SEQ ID NO:20, or SEQ ID NO:21,or SEQ ID NO: 22, or SEQ ID

NO:23, or SEQ ID NO:24, or SEQ ID NO:25, or SEQ ID NO:26, or SEQ ID NO:27, or SEQ ID NO:28, or SEQ ID NO:29, or SEQ ID NO:30, or SEQ ID NO: or SEQ ID NO:31, or SEQ ID NO:32,or SEQ ID NO: 33, or SEQ ID NO:34, or SEQ ID NO:35, or SEQ ID NO:36 , or SEQ ID NO:37, or SEQ ID NO:38, or SEQ ID NO: or SEQ ID NO:39, or SEQ ID NO:40, or SEQ ID NO:41, or SEQ ID NO:42.

The present invention further provides a method for identifying a protein having a bromodomain. One such embodiment comprises contacting a cellular extract with a peptide comprising an acetyl-lysine.

The present invention further provides agents that can inhibit the binding of a bromodomain with a protein comprising an acetyl-lysine. In one embodiment the agent is ISYGR-*AcK*-KRRQRR (SEQ ID NO:4). In another embodiment the agent is ARKSTGG-A*cK*-APRKQL (SEQ ID NO:5). In still another embodiment the agent is QSTSRHK-*AcK*-LMFKTE (SEQ ID NO:6). In yet another embodiment the agent is an analog of acetyl-lysine such as acetyl-histamine. In still another embodiment the agent is an antibody that recognizes an acetyl-lysine of a protein binding partner of a bromodomain. In a preferred embodiment the agent is an antibody raised against a ZA loop of a bromodomain. These agents can be used as pharmaceuticals in compositions that contain a pharmaceutically acceptable carrier for example, or in the various drug assays of the present invention, serving as controls to demonstrate specificity.

Accordingly, it is a principal object of the present invention to provide the three-dimensional coordinates of a bromodomain.

It is a further object of the present invention to provide the three-dimensional coordinates of a bromodomain complexed with acetyl-histamine.

It is a further object of the present invention to provide an assay for identifying proteins that contain bromodomains that bind proteins that comprise acetyl-lysine.

It is a further object of the present invention to provide methods of identifying drugs that can modulate the bromodomain-acetyl-lysine binding complex.

It is a further object of the present invention to provide methods of identifying drugs that can inhibit the binding of a bromodomain to a protein containing acetyl-lysine.

It is a further object of the present invention to provide methods that incorporate the use of rational design for identifying such drugs.

It is a further object of the present invention to provide a method of identifying drugs that can treat leukemia.

It is a further object of the present invention to provide a method of identifying drugs that can treat and/or prevent AIDS.

These and other aspects of the present invention will be better appreciated by reference to the following drawings and Detailed Description.

BRIEF DESCRIPTION OF THE DRAWINGS

Figure 1. Structure-based sequence alignment of a selected number of bromodomains. The sequences were aligned based on the NMR-derived structure of the P/CAF bromodomain, and the predicated four α-helices are shown in green boxes. Bromodomains are grouped on the basis of the sequence and/or functional similarities as described by Jeanmougin *et al.*, [Trends in Biochemical *Sciences*, **22:**151-153 (1997)]. Residue numbers of the P/CAF bromodomain are indicated above its sequence. Three absolutely conserved residues, corresponding to Pro751, Pro767, and Asn803 in the P/CAF bromodomain, are shown in red. Highly conserved residues are colored in blue. The residues of the P/CAF bromodomain that interact with acetyl-histamine, as determined by intermolecular NOEs, are indicated by asterisks. The ZA loop, which is critical for acetyl-lysine binding, for each of the indicated bromodomains is also identified. The underlined residues were changed individually

by site-directed mutagenesis to Ala. Genbank accession numbers for the proteins are as indicated in Table 8, in the Example below, along with the SEQ ID NOs. for the bromodomain sequences.

Figures 2A-2H depict the structure of the P/CAF bromodomain. Figures 2A-2B shows the stereoview of the C_α trace of 30 superimposed NMR-derived structures of the bromodomain (residues 722-830). The N-terminal four residues (SKEP) which are structurally disordered are omitted for clarity. For the final 30 structures, the root-mean-square deviations (RMSDs) of the backbone and all heavy atoms are 0.63 ± 0.11Å and 1.15 ± 0.12Å for residues 723-830, respectively. The RMSDs of the backbone and all heavy atoms for the four α-helices (residues 727-743, 770-776, 785-802, and 807-827), are 0.34 ± 0.04Å and 0.87 ± 0.06Å, respectively. Figures 2C-2D show the stereoview of the bromodomain structures from the bottom of the protein, which is rotated approximately 90° from the orientation in Figures 2A-2B. Figure 2E shows the Ribbons [Carson, M., *J. Appl. Crystallogr.* **24**:958-961 (1991)] depiction of the averaged minimized NMR structure of the P/CAF bromodomain. The orientation of Figure 2E is as shown in Figures 2A-2B. Figures 2F-2G are schematic representations of the overall topology of the up-and-down four-helix bundle folds with the opposite handedness. The left-handed fold is seen in bromodomain, cytochrome b_5, and T4 lysozyme (left, Figure 2F), whereas the right-handed four-helix bundles are observed in proteins such as hemerythrin and cytochrome b_{562} (right, Figure 2G) [Richardson, J., *Adv.Protein Chem.*, **34**:167-339 (1989); Presnell and Cohen, *Proc. Natl. Acad. Sci. USA* **86**:6592-6596 (1989)]. Figure 2H is a molecular surface representation of the electrostatic potential (blue = positive; red = negative) of the bromodomain calculated in GRASP [Nicholls *et al.*, *Biophys. J.* **64**:166-170 (1993)]. The hydrophobic and aromatic residues (Tyr809, Tyr802, Tyr760, Ala757, and Val752) located between the ZA and BC loops are indicated.

Figures 3A-3C show the binding of the P/CAF bromodomain to AcK. Figure 3A shows the superimposed region of the 2D ^{15}N-HSQC spectra of the bromodomain (approximately 0.5 mM) in its free form (red) and complexed to the AcK-containing

H4 peptide (molar ratio 1:6) (black). Figure 3B is the Ribbon and dotted-surface diagram of the bromodomain depicting the location of the lysine-acetylated H4 peptide binding site. The color coding reflects the chemical shift changes ($\Delta\delta$) of the backbone amide ^{1}H and ^{15}N resonances upon binding to the AcK peptide as observed in the ^{15}N-HSQC spectra. The normalized weighted average of the chemical shift changes was calculated by $\Delta_{av}/\Delta_{max} = [\Delta\delta^{2}_{NH} + \Delta\delta^{2}_{N}/25)/2]^{1/2}/\Delta_{max}$, where Δ_{max} is the maximum weighted chemical shift difference observed for Tyr809 (0.16ppm). The backbone atoms are color-coded in red, yellow, or green for residues that have Δ_{av}/Δ_{max} of >0.6 (Tyr809, Glu808, Asn803, and Ala757), 0.2-0.6 (Ala813, Tyr802, Tyr760, and Val752), or <0.2 (Cys812, Ser807, Cys799, Phe796, and Phe748), respectively. The non-perturbed residues are shown in blue. Figure 3C shows the chemical structures of acetyl-lysine, acetyl-histamine, and acetyl-histidine.

Figure 4 depicts the acetyl-lysine binding pocket. This is the Ribbons [Carson, M., *J. Appl. Crystallogr.* **24**:958-961 (1991)] depiction of a portion of the P/CAF bromodomain complexed with the acetyl-histamine. The ligand is color-coded by atom type.

DETAILED DESCRIPTION OF THE INVENTION

The present invention identifies a general binding partner (ligand) for the protein motif known as the bromodomain. Indeed, by combining structural and site-directed mutagenesis studies the present invention demonstrates that bromodomains can interact specifically with acetyl-lysine (AcK), making them the first protein modules known to exhibit such interactions. Like other modular domains, such as Src homology-2 (SH2) and phosphotyrosine binding (PTB) domains, which specifically interact with phosphotyrosine-containing proteins, the bromodomain/acetyl-lysine recognition provides a means to regulate protein-protein interactions via protein lysine acetylation. The nature of the acetyl-lysine recognition by the bromodomain is similar to that of histone acetyltransferase interaction with acetyl-CoA. The present invention therefore couples for the first time, the functionality of the bromodomain with the HAT activity of coactivators in the regulation of gene transcription.

The present invention further provides both a nuclear magnetic resonance (NMR) structure of the bromodomain from the HAT coactivator P/CAF (p300/CBP-associated factor) as well as the structure for the P/CAF bromodomain in complex with acetyl-histamine. The structure reveals an unusual left-handed up-and-down four-helix bundle.

The results disclosed herein explain prior deletion experiments which showed that the bromodomain is indispensable for the function of GCN5 in yeast. Bromodomain-AcK binding also appears to be important for the assembly and activity of multiprotein complexes in transcriptional activation. The results reported herein therefore, form the foundation for identifying specific biological ligands and for defining the molecular mechanisms by which the extensive family of bromodomains participate in chromatin remodeling and transcriptional activation

As disclosed herein, the binding partner for the bromodomain is a peptide or protein comprising an acetyl-lysine (AcK). Interestingly, whereas a free acetyl-lysine does not appear to bind the bromodomain, an analog of the acetyl-lysine, acetyl-histamine, does. This is most likely due to the additional charge present in the free amino acid. Consistently, free acetyl-histidine also does not to bind the bromodomain.

The present invention further provides a key region of the bromodomain for the interaction with its acetyl-lysine binding partner, the ZA loop. The amino acid sequence of the ZA loop is defined in Figure 1 for a number of bromodomains and is depicted in Figure 2A for P/CAF. In a particular embodiment, the ZA loop has between about 21 and 40 amino acid residues comprising the amino acid sequence of :

$$F\ X_{2\text{-}3}\ P\ X_{5\text{-}8}\ J_{P/K/H}\ X\ Y\ J_{Y/F/H}\ X_5\ P\ J_{M/I/V}\ D \qquad \text{(SEQ ID NO:3)}$$

more preferably the ZA loop has about 23 to 34 amino acid residues and comprises the amino acid sequence:

$$X_2\ F\ X_{2\text{-}3}\ P\ X_{5\text{-}8}\ J_{P/K/H}\ X\ Y\ J_{Y/F/H}\ X_5\ P\ J_{M/I/V}\ D \qquad \text{(SEQ ID NO:43)}$$

(1) The single letter amino acid code is used in this description, *i.e.*,"F" for phenylalanine; "P" for proline; "Y" for tyrosine; and "D" for aspartic acid.

(2) "X" indicates any amino acid (an undesignated amino acid); and X, X_2, X_{2-3}, X_5,and X_{5-8} indicates one undesignated amino acid, two consecutive undesignated amino acids, two or three consecutive undesignated amino acids, five consecutive undesignated amino acids, and five to eight consecutive undesignated amino acids respectively.

(3) "J" indicates that identity of the amino acid is restricted to a particular group, again the one letter code is used

: (i) $J_{P/K/H}$ is either proline, lysine or histidine.

(ii) $J_{Y/F/H}$ is either tyrosine, phenylalanine or histidine.

(iii) $J_{M/I/V}$ is either methionine, isoleucine, or valine.

Since this region of the bromodomain is important in binding its acetyl-lysine binding partner, antibodies specifically raised against this region are also included in the present invention. In a particular embodiment, the antibody is a humanized chimeric antibody that can be used in therapeutic treatment. Thus monoclonal, chimeric, and polyclonal antibodies raised against bromodomains, preferably against amino acid residues in the ZA loop region are part of the present invention. In a specific embodiment the antibody is raised against a peptide, fusion peptide or conjugated peptide consisting of amino acid residues 746 to 765 of SEQ ID NO:2, *i.e.*, WPFMEPVKRTEAPGYYEVIR (SEQ ID NO:44). Such antibodies can be used in the treatment of leukemia for example. Alternatively, these antibodies can be used in drug discovery assays.

Thus the present invention provides the first detailed structural information regarding a bromodomain and a bromodomain complexed with its acetylated binding partner. The present invention therefore provides the three-dimensional structure of the bromodomain and a bromodomain acetylated binding partner complex. Since the interaction of the bromodomain with a histone for example, can play a significant role in chromatin remodeling/regulation, the structural information provided herein can be employed in methods of identifying drugs that can modulate basic cell processes by modulating the transcription. In a particular embodiment, the three-dimensional

structural information is used in the design of a small organic molecule for the treatment of cancer.

Indeed, the bromodomain and lysine-acetylated protein interaction can now be implicated to play a causal role in the development of a number of diseases including cancers such as leukemia. For example, chromatin remodeling plays a central role in the etiology of viral infection and cancer [Archer and Hodin, *Curr. Opin. Genet. Biol.* **9**:171-174 (1999); Jacobson and Pillus, *Curr. Opin. Genet. Biol.* **9**:175-184 (1999)]. Both altered histone acetylation/deacetylation and aberrant forms of chromatin-remodeling complexes are associated with human diseases. Furthermore, chromosomal translocation of various cellular genes with those encoding HATs and subunits of chromatin remodeling complexes have been implicated in leukomogenesis. The *MOZ* (monocytic leukemia zinc finger) and *MLL/ALL-1* genes are frequently fused to the gene encoding the co-activator HAT CBP [Sobulo *et al.*, *Proc. Natl. Acad. Sci. USA* **94**:8732-8737(1997)]. The resulting fusion protein MLL-CBP contains the tandem bromodomain-PHD finger-HAT domain of CBP. It also has been shown that both the bromodomain and HAT domain of CBP are required for leukomogenesis, because deletion of either the bromodomain or the HAT domain results in loss of the MLL-CBP fusion protein's ability for cell transform. These results indicate that the CBP bromodomain, and more particularly, the ZA loop of the CBP bromodomain, is an excellent target for developing drugs that interfere with the bromodomain acetyl-lysine interaction that can be used in the treatment of human acute leukemia. In addition, an antibody (*e.g.*, a humanized antibody) raised specifically against a peptide from the ZA loop of the CBP bromodomain could also be effective for treating these conditions.

Furthermore, the human immunodeficiency virus type 1 (HIV-1) *trans*-activator protein, Tat, is absolutely required for productive HIV viral replication [Jeang and Gatignol, *Curr. Top. Microbiol. Immunol.*, **188**:123-144(1994)]. Recently, it has been shown that HIV-1 Tat transcriptional activity is tightly regulated by lysine acetylation [Kiernan *et al.*, *EMBO Journal* **18**:6106-6118 (1999)]. Therefore, the interaction of the acetyl-lysine of Tat with one or more bromodomain-containing proteins associated

with chromatin remodeling could mediate gene transcription. Thus, the bromodomain/lysine-acetylated Tat interaction could also serve as a drug target for blocking HIV replication in cells. Similarly, an antibody raised specifically against a peptide from the ZA loop of the bromodomain could also be effective for treating these conditions.

In addition, based on the new structural information disclosed herein, the key amino acid residues for the binding of a given bromodomain and its binding partner can be identified and further elucidated using basic mutagenesis and standard isothermal titration calorimetry, for example. In this case, both the crucial amino acids for the bromodomain and the binding partner (i.e., apart from the acetyl-lysine) can be readily determined and are also part of the present invention.

The results obtained from the structural and functional studies disclosed herein provide the foundation for both high throughput drug screening and structure-based rational drug design. The agents identified by this procedure will be useful for ameliorating conditions involving chromatin remodeling/regulation as indicated above.

Structure based rational drug design is the most efficient method of drug development. However, heretofore, no information has been disclosed regarding the structure of the bromodomain or more importantly, its interaction with the acetyl-lysine of its binding partner. Obtaining detailed structural information requires an extensive NMR or X-ray crystallographic analysis. By determining and then exploiting the detailed structural information of the bromodomain and of the bromodomain/acetyl-histamine (exemplified by NMR analysis below) the present invention provides novel methods for developing new drugs through structure based rational drug design.

Thus the present invention provides representative sets of the atomic structure coordinates of the free form of the P/CAF bromodomain (Table 5) and of the P/CAF bromodomain-acetyl-histamine complex (Table 6) which were both obtained by NMR analysis. A Ribbon diagram of the three-dimensional structure of the P/CAF bromodomain is depicted in Figure 2E, whereas the P/CAF bromodomain acetyl-lysine

binding pocket is depicted in Figure 4. The present invention also provides the NOE-derived distance restraints, and NMR chemical shift assignments of the P/CAF bromodomain. The NMR chemical shift assignments of the P/CAF bromodomain are included in the chemical shift table (Table 1) for the ^{1}H-^{15}N HSQC spectrum of P/CAF bromodomain. The unambiguous NOE-derived Inter-proton Distance Restraints (Table 2), the ambiguous NOE-derived Inter-proton Distance Restraints (Table 3) and the ^{1}H bonding restraints (Table 4) are also disclosed herein. The sample atomic coordinate data provided enable the skilled artisan to practice the invention. In addition, Tables 1-6 are also capable of being placed into a computer readable form which is also part of the present invention. Furthermore, methods of using these coordinates and chemical shifts and related information (including in computer readable forms) either individually or together in drug assays are also provided. More particularly, such atomic coordinates can be used to identify potential ligands or drugs which will modulate the binding of a bromodomain with its binding partner.

Therefore, if appearing herein, the following terms shall have the definitions set out below.

As used herein a "bromodomain-acetyl-lysine binding complex" is a binding complex between a bromodomain or fragment thereof and either a peptide/polypeptide comprising an acetyl-lysine (or an analog of acetyl-lysine), or a free analog of acetyl-lysine, such as acetyl-histamine disclosed in the Example below. Preferably, the peptide comprises at least six amino acids in addition to the acetyl-lysine. The dissociation constant of a bromodomain-acetyl-lysine binding complex is dependent on whether the lysine residue or analog thereof is acetylated or not, such that the affinity for the bromodomain and the peptide comprising the lysine residue (for example) significantly decreases when that lysine residue is not acetylated.

As used herein a "ZA loop" of a bromodomain is one protion of a bromodomain that is involved in the binding of the bromodomain to the acetyl-lysine. The structure of the ZA loop of the bromodomain of for P/CAF is depicted in Figure 2A. The ZA loop has between about 20 and 40 amino acids and comprises the amino acid sequence of SEQ ID NO:3. More preferably the ZA loop comprises between about 23 to 34 amino acids

and has the amino acid sequence SEQ ID NO:43. The amino acid sequence of the ZA loop for a representative number of individual bromodomains is shown in Figure 1.

A "polypeptide" or "peptide" comprising a fragment of a bromodomain, such as the ZA loop, or a peptide or polypeptide comprising an acetyl-lysine, as used herein can be the "fragment" alone, or a larger chimeric or fusion peptide/protein which contains the "fragment".

As used herein the terms "fusion protein" and "fusion peptide" are used interchangeably and encompass "chimeric proteins and/or chimeric peptides" and fusion "intein proteins/peptides". A fusion protein comprises at least a portion of a protein or peptide of the present invention, *e.g.*, a bromodomain, joined *via* a peptide bond to at least a portion of another protein or peptide including *e.g.*, a second bromodomain in a chimeric fusion protein. In a particular embodiment the portion of the bromodomain is antigenic. Fusion proteins can comprise a marker protein or peptide, or a protein or peptide that aids in the isolation and/or purification of the protein, for example.

As used herein, and unless otherwise specified, the terms "agent", "potential drug", "compound", "test compound" or "potential compound" are used interchangeably, and refer to chemicals which potentially have a use as an inhibitor or activator/stabilizer of bromodomain-acetyl-lysine binding. Therefore, such "agents", "potential drugs", "compounds" and "potential compounds" may be used, as described herein, in drug assays and drug screens and the like.

As used herein a "small organic molecule" is an organic compound, including a peptide [or organic compound complexed with an inorganic compound (*e.g.*, metal)] that has a molecular weight of less than 3 Kilodaltons. Such small organic molecules can be included as agents, etc. as defined above.

As used herein the term "binds to" is meant to include all such specific interactions that result in two or more molecules showing a preference for one another relative to some third molecule. This includes processes such as covalent, ionic, hydrophobic and

hydrogen bonding but does not include non-specific associations such as solvent preferences.

As used herein the term "about" signifies that a value is within twenty percent of the indicated value *i.e.*, a peptide containing "about" 20 amino acid residues can contain between 16 and 24 amino acid residues.

General Techniques for Constructing Nucleic Acids That Encode the Bromodomains and Fragments Thereof (Incuding, ZA Loops); and the Bromodomain Binding Partners of the Present Invention.

In accordance with the present invention there may be employed conventional molecular biology, microbiology, and recombinant DNA techniques within the skill of the art. Such techniques are explained fully in the literature. See, *e.g.*, Sambrook, Fritsch & Maniatis, *Molecular Cloning: A Laboratory Manual,* Second Edition (1989) Cold Spring Harbor Laboratory Press, Cold Spring Harbor, New York (herein "Sambrook *et al.*, 1989"); *DNA Cloning: A Practical Approach,* Volumes I and II (D.N. Glover ed. 1985); *Oligonucleotide Synthesis* (M.J. Gait ed. 1984); *Nucleic Acid Hybridization* [B.D. Hames & S.J. Higgins eds. (1985)]; *Transcription And Translation* [B.D. Hames & S.J. Higgins, eds. (1984)]; *Animal Cell Culture* [R.I. Freshney, ed. (1986)]; *Immobilized Cells And Enzymes* [IRL Press, (1986)]; B. Perbal, *A Practical Guide To Molecular Cloning* (1984); F.M. Ausubel *et al.* (eds.), *Current Protocols in Molecular Biology*, John Wiley & Sons, Inc. (1994).

Therefore, if appearing herein, the following terms shall have the definitions set out below.

As used herein, the term "gene" refers to an assembly of nucleotides that encode a polypeptide, and includes cDNA and genomic DNA nucleic acids.

A "vector" is a replicon, such as plasmid, phage or cosmid, to which another DNA segment may be attached so as to bring about the replication of the attached segment. A "replicon" is any genetic element (e.g., plasmid, chromosome, virus) that functions

as an autonomous unit of DNA replication *in vivo*, *i.e.*, capable of replication under its own control.

A "cassette" refers to a segment of DNA that can be inserted into a vector at specific restriction sites. The segment of DNA encodes a polypeptide of interest, and the cassette and restriction sites are designed to ensure insertion of the cassette in the proper reading frame for transcription and translation.

A cell has been "transfected" by exogenous or heterologous DNA when such DNA has been introduced inside the cell.

A "nucleic acid molecule" refers to the phosphate ester polymeric form of ribonucleosides (adenosine, guanosine, uridine or cytidine; "RNA molecules") or deoxyribonucleosides (deoxyadenosine, deoxyguanosine, deoxythymidine, or deoxycytidine; "DNA molecules"), or any phosphoester analogues thereof, such as phosphorothioates and thioesters, in either single stranded form, or a double-stranded helix. Double stranded DNA-DNA, DNA-RNA and RNA-RNA helices are possible. The term nucleic acid molecule, and in particular DNA or RNA molecule, refers only to the primary and secondary structure of the molecule, and does not limit it to any particular tertiary forms. Thus, this term includes double-stranded DNA found, *inter alia*, in linear or circular DNA molecules (*e.g.*, restriction fragments), plasmids, and chromosomes. In discussing the structure of particular double-stranded DNA molecules, sequences may be described herein according to the normal convention of giving only the sequence in the 5′ to 3′ direction along the nontranscribed strand of DNA (*i.e.*, the strand having a sequence homologous to the mRNA). A "recombinant DNA molecule" is a DNA molecule that has undergone a molecular biological manipulation.

A nucleic acid molecule is "hybridizable" to another nucleic acid molecule, such as a cDNA, genomic DNA, or RNA, when a single stranded form of the nucleic acid molecule can anneal to the other nucleic acid molecule under the appropriate conditions of temperature and solution ionic strength (*see* Sambrook *et al.*, *supra*). The conditions of temperature and ionic strength determine the "stringency" of the

hybridization. For preliminary screening for homologous nucleic acids, low stringency hybridization conditions, corresponding to a T_m of 55°, can be used, *e.g.*, 5x SSC, 0.1% SDS, 0.25% milk, and no formamide; or 30% formamide, 5x SSC, 0.5% SDS). Moderate stringency hybridization conditions correspond to a higher T_m, *e.g.*, 40% formamide, with 5x or 6x SCC. High stringency hybridization conditions correspond to the highest T_m, *e.g.*, 50% formamide, 5x or 6x SCC. Hybridization requires that the two nucleic acids contain complementary sequences, although depending on the stringency of the hybridization, mismatches between bases are possible. The appropriate stringency for hybridizing nucleic acids depends on the length of the nucleic acids and the degree of complementation, variables well known in the art. The greater the degree of similarity or homology between two nucleotide sequences, the greater the value of T_m for hybrids of nucleic acids having those sequences. The relative stability (corresponding to higher T_m) of nucleic acid hybridizations decreases in the following order: RNA:RNA, DNA:RNA, DNA:DNA. For hybrids of greater than 100 nucleotides in length, equations for calculating T_m have been derived (*see* Sambrook *et al.*, *supra*, 9.50-10.51). For hybridization with shorter nucleic acids, *i.e.*, oligonucleotides, the position of mismatches becomes more important, and the length of the oligonucleotide determines its specificity (*see* Sambrook *et al.*, *supra*, 11.7-11.8). Preferably a minimum length for a hybridizable nucleic acid is at least about 12 nucleotides; preferably at least about 18 nucleotides; and more preferably the length is at least about 27 nucleotides; and most preferably 36 nucleotides.

In a specific embodiment, the term "standard hybridization conditions" refers to a T_m of 55°C, and utilizes conditions as set forth above. In a preferred embodiment, the T_m is 60°C; in a more preferred embodiment, the T_m is 65°C.

A DNA "coding sequence" is a double-stranded DNA sequence which is transcribed and translated into a polypeptide in a cell *in vitro* or *in vivo* when placed under the control of appropriate regulatory sequences. The boundaries of the coding sequence are determined by a start codon at the 5′ (amino) terminus and a translation stop codon at the 3′ (carboxyl) terminus. A coding sequence can include, but is not limited to, prokaryotic sequences and synthetic DNA sequences. If the coding sequence is

intended for expression in a eukaryotic cell, a polyadenylation signal and transcription termination sequence will usually be located 3′ to the coding sequence.

Transcriptional and translational control sequences are DNA regulatory sequences, such as promoters, enhancers, terminators, and the like, that provide for the expression of a coding sequence in a host cell. In eukaryotic cells, polyadenylation signals are control sequences.

A "promoter sequence" is a DNA regulatory region capable of binding RNA polymerase in a cell and initiating transcription of a downstream (3′ direction) coding sequence. For purposes of defining the present invention, the promoter sequence is bounded at its 3′ terminus by the transcription initiation site and extends upstream (5′ direction) to include the minimum number of bases or elements necessary to initiate transcription at levels detectable above background. Within the promoter sequence will be found a transcription initiation site (conveniently defined for example, by mapping with nuclease S1), as well as protein binding domains (consensus sequences) responsible for the binding of RNA polymerase.

A coding sequence is "under the control" of transcriptional and translational control sequences in a cell when RNA polymerase transcribes the coding sequence into mRNA, which is then trans-RNA spliced and translated into the protein encoded by the coding sequence.

A DNA sequence is "operatively linked" to an expression control sequence when the expression control sequence controls and regulates the transcription and translation of that DNA sequence. The term "operatively linked" includes having an appropriate start signal (e.g., ATG) in front of the DNA sequence to be expressed and maintaining the correct reading frame to permit expression of the DNA sequence under the control of the expression control sequence and production of the desired product encoded by the DNA sequence. If a gene that one desires to insert into a recombinant DNA molecule does not contain an appropriate start signal, such a start signal can be inserted in front of the gene.

As used herein, the term "homologous" in all its grammatical forms refers to the relationship between proteins that possess a "common evolutionary origin," including proteins from superfamilies (*e.g.*, the immunoglobulin superfamily) and homologous proteins from different species (*e.g.*, myosin light chain, etc.) [Reeck *et al., Cell,* **50:**667 (1987)]. Such proteins have sequence homology as reflected by their high degree of sequence similarity.

Accordingly, the term "sequence similarity" in all its grammatical forms refers to the degree of identity or correspondence between nucleic acid or amino acid sequences of proteins that may or may not share a common evolutionary origin (*see* Reeck *et al.*, *supra*). However, in common usage and in the instant application, the term "homologous," when modified with an adverb such as "highly," may refer to sequence similarity and not a common evolutionary origin.

Two DNA sequences are "substantially homologous" when at least about 60% (preferably at least about 80%, and most preferably at least about 90 or 95%) of the nucleotides match over the defined length of the DNA sequences. Sequences that are substantially homologous can be identified by comparing the sequences using standard software available in sequence data banks, or in a Southern hybridization experiment under, for example, stringent conditions as defined for that particular system. Defining appropriate hybridization conditions is within the skill of the art. See, e.g., Maniatis et al., *supra*; DNA Cloning, Vols. I & II, *supra*; Nucleic Acid Hybridization, *supra*.

As used herein an amino acid sequence is 100% "homologous" to a second amino acid sequence if the two amino acid sequences are identical, and/or differ only by neutral or conservative substitutions as defined below. Accordingly, an amino acid sequence is 50% "homologous" to a second amino acid sequence if 50% of the two amino acid sequences are identical, and/or differ only by neutral or conservative substitutions.

As used herein, DNA and protein sequence percent identity can be determined using MacVector 6.0.1, Oxford Molecular Group PLC (1996) and the Clustal W algorithm with the alignment default parameters, and default parameters for identity. These

commercially available programs can also be used to determine sequence similarity using the same or analogous default parameters.

The term "corresponding to" is used herein to refer similar or homologous sequences, whether the exact position is identical or different from the molecule to which the similarity or homology is measured. Thus, the term "corresponding to" refers to the sequence similarity, and not the numbering of the amino acid residues or nucleotide bases.

As used herein a "heterologous nucleotide sequence" is a nucleotide sequence that is added to a nucleotide sequence of the present invention by recombinant methods to form a nucleic acid which is not naturally formed in nature. Such nucleic acids can encode fusion proteins or peptides, including chimeric proteins and peptides. Thus the heterologous nucleotide sequence can encode peptides and/or proteins which contain regulatory and/or structural properties. In another such embodiment the heterologous nucleotide can encode a protein or peptide that functions as a means of detecting the protein or peptide encoded by the nucleotide sequence of the present invention after the recombinant nucleic acid is expressed. In still another such embodiment the heterologous nucleotide can function as a means of detecting a nucleotide sequence of the present invention. A heterologous nucleotide sequence can comprise non-coding sequences including restriction sites, regulatory sites, promoters and the like.

The present invention also relates to cloning vectors containing nucleic acids encoding analogs and derivatives of the bromodomains of the present invention and polypeptides/peptides that can bind a bromodomain when a lysine of the polypeptide/peptide is acetylated, including modified fragments, that have the same or homologous functional activity as the individual fragments, and homologs thereof. The production and use of derivatives and analogs related to the fragments are within the scope of the present invention.

Due to the degeneracy of nucleotide coding sequences, other DNA sequences which encode substantially the same amino acid sequence as a nucleic acid encoding a protein

comprising bromodomain or bromodomain binding partner (*i.e.*, when post-transcriptionally acetylated) of the present invention for example, may be used in the practice of the present invention. These include but are not limited to allelic genes, homologous genes from other species, which are altered by the substitution of different codons that encode the same amino acid residue within the sequence, thus producing a silent change. Likewise, the peptides and polypeptides of the present invention include, but are not limited to, those containing, as a primary amino acid sequence, analogous portions of their respective amino acid sequences including altered sequences in which functionally equivalent amino acid residues are substituted for residues within the sequence resulting in a conservative amino acid substitution. For example, one or more amino acid residues within the sequence can be substituted by another amino acid of a similar polarity, which acts as a functional equivalent, resulting in a silent alteration. Substitutes for an amino acid within the sequence may be selected from other members of the class to which the amino acid belongs. For example, the nonpolar (hydrophobic) amino acids include alanine, leucine, isoleucine, valine, proline, phenylalanine, tryptophan and methionine. Amino acids containing aromatic ring structures are phenylalanine, tryptophan, and tyrosine. The polar neutral amino acids include glycine, serine, threonine, cysteine, tyrosine, asparagine, and glutamine. The positively charged (basic) amino acids include arginine, and lysine. The negatively charged (acidic) amino acids include aspartic acid and glutamic acid.

Particularly preferred conserved amino acid exchanges are:

(a) Lys for Arg or vice versa such that a positive charge may be maintained;

(b) Glu for Asp or vice versa such that a negative charge may be maintained;

(c) Ser for Thr or vice versa such that a free -OH can be maintained;

(d) Gln for Asn or vice versa such that a free NH_2 can be maintained;

(e) Ile for Leu or for Val or vice versa as roughly equivalent hydrophobic amino acids; and

(f) Phe for Tyr or vice versa as roughly equivalent aromatic amino acids.

A conservative change generally leads to less change in the structure and function of the resulting protein. A non-conservative change is more likely to alter the structure,

activity or function of the resulting protein. The present invention should be considered to include sequences containing conservative changes which do not significantly alter the activity or binding characteristics of the resulting protein. Specific amino acid residues for the P/CAF bromodomain have been identified that are important for binding, indicating a potential lower stringency for the substitution of the remaining amino acids residues.

All of the peptides/fragments of the present invention can be modified by being placed in a fusion or chimeric peptide or protein, or labeled *e.g.*, to have an N-terminal FLAG-tag, or H6 tag. In a particular embodiment the P/CAF bromodomain fragment can be modified to contain a marker protein such as green fluorescent protein as described in U.S. Patent No. 5,625,048 filed April 29, 1997 and WO 97/26333, published July 24, 1997 each of which are hereby incorporated by reference herein in their entireties.

The nucleic acids encoding peptides and protein fragments of the present invention and analogs thereof can be produced by various methods known in the art. The manipulations which result in their production can occur at the gene or protein level [Sambrook *et al.*, 1989, *supra*]. The nucleotide sequence can be cleaved at appropriate sites with restriction endonuclease(s), followed by further enzymatic modification if desired, isolated, and ligated *in vitro*. In addition a nucleic acid sequence can be mutated *in vitro* or *in vivo*, to create and/or destroy translation, initiation, and/or termination sequences, or to create variations in coding regions and/or form new restriction endonuclease sites or destroy preexisting ones, to facilitate further *in vitro* modification. Any technique for mutagenesis known in the art can be used, including but not limited to, *in vitro* site-directed mutagenesis [Hutchinson *et al.*, *J. Biol. Chem.*, **253**:6551 (1978); Zoller and Smith, *DNA,* **3**:479-488 (1984); Oliphant *et al.*, *Gene,* **44**:177 (1986); Hutchinson *et al.*, *Proc. Natl. Acad. Sci. U.S.A.*, **83**:710 (1986)], use of TAB® linkers (Pharmacia), etc. PCR techniques are preferred for site directed mutagenesis [see Higuchi, 1989, "Using PCR to Engineer DNA", in *PCR Technology: Principles and Applications for DNA Amplification*, H. Erlich, ed., Stockton Press, Chapter 6, pp. 61-70].

The identified and isolated nucleic acids can then be inserted into an appropriate cloning vector. A large number of vector-host systems known in the art may be used.

Protein expression and purification

A bacterial protein expression system can be used to make various stable isotopically labeled (^{13}C, ^{15}N, and ^{2}H) protein samples that are useful for a three-dimensional NMR structural determination of a protein complex. For example a pET14b (Novagen) bacterial expression vector can be constructed which expresses the recombinant P/CAF bromodomain as an amino-terminal His-tagged fusion protein.

Protein expression and purification can be conducted using standard procedures for His-tagged proteins [Zhou *et al.*, *J. Biol. Chem.* **270**:31119-31123 (1995)]. To optimize the level of protein expression, various bacterial growth and expression conditions can be screened, which include different *E. Coli* cell lines, and growth and protein induction temperatures. Generally, it is preferred to obtain the maximum amount of soluble protein while still inducing protein expression with a relatively low IPTG concentration *e.g.*, ~0.2mM (final concentration) at 16°C. As exemplified below, the bromodomain of P/CAF (residues 719-832 of SEQ ID NO:2 which is SEQ ID NO:7) was subcloned into the pET14b expression vector (Novagen) and expressed in *Escherichia coli* BL21(DE3) cells. Uniformly ^{15}N- and $^{15}N/^{13}C$-labeled proteins were prepared by growing bacteria in a minimal medium containing $^{15}NH_4Cl$ with or without $^{13}C_6$-glucose. A uniformly $^{15}N/^{13}C$-labeled and fractionally deuterated protein sample was prepared by growing the cells in 75% $^{2}H_2O$. The bromodomain was purified by affinity chromatography on a nickel-IDA column (Invitrogen) followed by the removal of poly-His tag by thrombin cleavage. The final purification of the protein was achieved by size-exclusion chromatography. The acetyl-lysine-containing peptides were prepared on a MilliGen 9050 peptide synthesizer (Perkin Elmer) using Fmoc/HBTU chemistry. Acetyl-lysine was incorporated using the reagent Fmoc-Ac-Lys with HBTU/DIPEA activation. NMR samples contained approximately 1 mM protein in 100mM phosphate buffer of pH 6.5 and 5mM perdeuterated DTT and 0.5mM EDTA in $H_2O/^{2}H_2O$ (9/1) or $^{2}H_2O$.

One major advantage of using the heteronuclear multidimensional approach, as exemplied herein, is that the NMR resonance assignments of a protein are obtained in a sequence-specific manner which assures accuracy and greatly facilitates data analysis and structure determination [Clore, G. M. & Gronenborn, A. M. *Meth. Enzymol.* **239:**249-363 (1994)]. In addition, the signal overlapping problems in the protein spectra are minimized by the use of multidimensional NMR spectra, which separates the proton signals according to the chemical shifts of their attached hetero-nuclei (such as ^{15}N and ^{13}C). This NMR approach has been proven very powerful for structural analysis of large proteins [Clore, G. M. & Gronenborn, A. M. *Meth. Enzymol.* **239:**249-363 (1994)]. To facilitate sequence-specific resonance assignments for the structural study, a uniformly ^{13}C, ^{15}N-labeled and fractionally (75%) deuterated protein sample of the bromodomain can be prepared by growing bacterial cells in 75% $^{2}H_2O$ as exemplified below. Such protein samples can be used for triple-resonance NMR experiments. A triple-labeled protein sample is useful for high-resolution NMR structural studies. Because of the favorable ^{1}H, ^{13}C, and ^{15}N relaxation rates caused by the partial deuteration of the protein, constant-time triple-resonance NMR spectra can be acquired with higher digital resolution and sensitivity [Sattler, M. & Fesik, S. W. *Structure* **4**:1245-1249 (1996)]. In addition, various stable-isotopically labeled (^{15}N and ^{13}C /^{15}N) proteins can also be prepared using this procedure.

Synthetic Polypeptides

The term "polypeptide" is used in its broadest sense to refer to a compound of two or more subunit amino acids, amino acid analogs, or peptidomimetics. The subunits are linked by peptide bonds. The terms "polypeptide", "protein", and "peptide" are used interchangeably herein, though preferably as used herein a "peptide" refers to a compound of at least two but less than fifty subunit amino acids, and a polypeptide or protein refers to compound of fifty or more amino acids. The polypeptides of the present invention may be chemically synthesized or as detailed above, genetically engineered or isolated from natural sources.

In addition, potential drugs or agents that may be tested in the drug screening assays of the present invention may also be chemically synthesized. When the peptide is to be

modified, *e.g.*, acetylated, the modification can be at any time during the peptide synthesis, including using an acetyl-lysine as a starting material or acetylating a lysine residue of a peptide after the peptide has been synthesized. In the Example below, the acetyl-lysine-containing peptides were prepared on a MilliGen 9050 peptide synthesizer (Perkin Elmer) using Fmoc/HBTU chemistry. Acetyl-lysine was incorporated using the reagent Fmoc-Ac-Lys with HBTU/DIPEA activation.

Thus, synthetic polypeptides, prepared using the well known techniques of solid phase, liquid phase, or peptide condensation techniques, or any combination thereof, can include natural and unnatural amino acids. Amino acids used for peptide synthesis may be standard Boc (N^{α}-amino protected N^{α}-t-butyloxycarbonyl) amino acid resin with the standard deprotecting, neutralization, coupling and wash protocols of the original solid phase procedure of Merrifield [*J. Am. Chem. Soc.*, **85:**2149-2154 (1963)], or the base-labile N^{α}-amino protected 9-fluorenylmethoxycarbonyl (Fmoc) amino acids first described by Carpino and Han [*J. Org. Chem.*, **37:**3403-3409 (1972)]. Both Fmoc and Boc N^{α}-amino protected amino acids can be obtained from Fluka, Bachem, Advanced Chemtech, Sigma, Cambridge Research Biochemical, Bachem, or Peninsula Labs or other chemical companies familiar to those who practice this art. In addition, the method of the invention can be used with other N^{α}-protecting groups that are familiar to those skilled in this art. Solid phase peptide synthesis may be accomplished by techniques familiar to those in the art and provided, for example, in Stewart and Young [Solid Phase Synthesis, Second Edition, Pierce Chemical Co., Rockford, IL (1984)] and Fields and Noble [*Int. J. Pept. Protein Res.*, **35:**161-214 (1990)], or using automated synthesizers, such as sold by ABS. Thus, polypeptides of the invention may comprise D-amino acids, a combination of D- and L-amino acids, and various "designer" amino acids (*e.g.*, β-methyl amino acids, Cα-methyl amino acids, and Nα-methyl amino acids, etc.) to convey special properties. Synthetic amino acids include ornithine for lysine, fluorophenylalanine for phenylalanine, and norleucine for leucine or isoleucine. Additionally, by assigning specific amino acids at specific coupling steps, α-helices, β turns, β sheets, γ-turns, and cyclic peptides can be generated.

In a further embodiment, subunits of peptides that confer useful chemical and structural properties will be chosen. For example, peptides comprising D-amino acids will be resistant to L-amino acid-specific proteases *in vivo*. In addition, the present invention envisions preparing peptides that have more well defined structural properties, and the use of peptidomimetics, and peptidomimetic bonds, such as ester bonds, to prepare peptides with novel properties. In another embodiment, a peptide may be generated that incorporates a reduced peptide bond, i.e., R_1-**CH_2-NH**-R_2, where R_1 and R_2 are amino acid residues or sequences. A reduced peptide bond may be introduced as a dipeptide subunit. Such a molecule would be resistant to peptide bond hydrolysis, *e.g.*, protease activity. Such peptides would provide ligands with unique function and activity, such as extended half-lives *in vivo* due to resistance to metabolic breakdown, or protease activity. Furthermore, it is well known that in certain systems constrained peptides show enhanced functional activity [Hruby, *Life Sciences,* **31:**189-199 (1982); Hruby *et al.*, *Biochem J.,* **268:**249-262 (1990)]; the present invention provides a method to produce a constrained peptide that incorporates random sequences at all other positions.

Constrained and cyclic peptides. A constrained, cyclic or rigidized peptide may be prepared synthetically, provided that in at least two positions in the sequence of the peptide an amino acid or amino acid analog is inserted that provides a chemical functional group capable of crosslinking to constrain, cyclise or rigidize the peptide after treatment to form the crosslink. Cyclization will be favored when a turn-inducing amino acid is incorporated. Examples of amino acids capable of crosslinking a peptide are cysteine to form disulfides, aspartic acid to form a lactone or a lactam, and a chelator such as γ-carboxyl-glutamic acid (Gla) (Bachem) to chelate a transition metal and form a cross-link. Protected γ-carboxyl glutamic acid may be prepared by modifying the synthesis described by Zee-Cheng and Olson [*Biophys. Biochem. Res. Commun.,* **94:**1128-1132 (1980)]. A peptide in which the peptide sequence comprises at least two amino acids capable of crosslinking may be treated, *e.g.*, by oxidation of cysteine residues to form a disulfide or addition of a metal ion to form a chelate, so as to crosslink the peptide and form a constrained, cyclic or rigidized peptide.

The present invention provides strategies to systematically prepare cross-links. For example, if four cysteine residues are incorporated in the peptide sequence, different protecting groups may be used (Hiskey, in The Peptides: Analysis, Synthesis, Biology, Vol. 3, Gross and Meienhofer, eds., Academic Press: New York, pp. 137-167 (1981); Ponsanti *et al.*, *Tetrahedron,* **46:**8255-8266 (1990)]. The first pair of cysteines may be deprotected and oxidized, then the second set may be deprotected and oxidized. In this way a defined set of disulfide cross-links may be formed. Alternatively, a pair of cysteines and a pair of chelating amino acid analogs may be incorporated so that the cross-links are of a different chemical nature.

Non-classical amino acids that induce conformational constraints. The following non-classical amino acids may be incorporated in the peptide in order to introduce particular conformational motifs: 1,2,3,4-tetrahydroisoquinoline-3-carboxylate [Kazmierski *et al.*, *J. Am. Chem. Soc.,* **113:**2275-2283 (1991)]; (2S,3S)-methyl-phenylalanine, (2S,3R)-methyl-phenylalanine, (2R,3S)-methyl-phenylalanine and (2R,3R)-methyl-phenylalanine (Kazmierski and Hruby, *Tetrahedron Lett.* (1991)]; 2-aminotetrahydronaphthalene-2-carboxylic acid [Landis, Ph.D. Thesis, University of Arizona (1989)]; hydroxy-1,2,3,4-tetrahydroisoquinoline-3-carboxylate [Miyake *et al.*, *J. Takeda Res. Labs.,* **43:**53-76 (1989)]; β-carboline (D and L) [Kazmierski, Ph.D. Thesis, University of Arizona (1988)]; HIC (histidine isoquinoline carboxylic acid) [Zechel *et al.*, *Int. J. Pep. Protein Res.,* 43 (1991)]; and HIC (histidine cyclic urea) (Dharanipragada).

The following amino acid analogs and peptidomimetics may be incorporated into a peptide to induce or favor specific secondary structures: LL-Acp (LL-3-amino-2-propenidone-6-carboxylic acid), a β-turn inducing dipeptide analog [Kemp *et al.*, *J. Org. Chem.,* **50:**5834-5838 (1985)]; β-sheet inducing analogs [Kemp *et al.*, *Tetrahedron Lett.,* **29:**5081-5082 (1988); β-turn inducing analogs [Kemp *et al.*, *Tetrahedron Lett.,* **29:**5057-5060 (1988)]; ∝-helix inducing analogs (Kemp *et al.*, *Tetrahedron Lett.,* **29:**4935-4938 (1988)]; γ-turn inducing analogs [Kemp *et al.*, *J. Org. Chem.,* **54:**109:115 (1989)]; and analogs provided by the following references: Nagai and Sato, *Tetrahedron Lett.,* **26:**647-650 (1985); DiMaio *et al.*, *J. Chem. Soc. Perkin Trans.,* p. 1687 (1989); also a Gly-Ala turn analog [Kahn *et al.*, *Tetrahedron*

Lett., **30**:2317 (1989)]; amide bond isostere [Jones *et al.*, *Tetrahedron Lett.*, **29**:3853-3856 (1988)]; tretrazol [Zabrocki *et al.*, *J. Am. Chem. Soc.*, **110**:5875-5880 (1988)]; DTC [Samanen *et al.*, *Int. J. Protein Pep. Res.*, **35**:501:509 (1990)]; and analogs taught in Olson *et al.*, *J. Am. Chem. Sci.*, **112**:323-333 (1990) and Garvey *et al.*, *J. Org. Chem.*, **56**:436 (1990). Conformationally restricted mimetics of beta turns and beta bulges, and peptides containing them, are described in U.S. Patent No. 5,440,013, issued August 8, 1995 to Kahn.

Structure-based Mutation Analysis

Protein structural analysis using NMR spectroscopy has several unique advantages. In addition to high-resolution three-dimensional structural information, the chemical shift assignments for the protein obtained in the structural study further provides a map of the entire protein at the atomic level, which can be used for structure-based biochemical analysis of protein-protein interactions. For example, the information generated from the NMR structural analysis can also serve to identify specific amino acid residues in the peptide-binding site for complementary mutagenesis studies. Specific focus can be placed on those residues that display long-range NOEs (particularly the side-chain NOEs in the ^{13}C-NOESY data) between the bromoomain and a peptide comprising an acetyl-lysine.

To ensure mutant proteins are valid for functional analysis, it can be determined as to whether a mutation results in any significant perturbation of the overall conformation of the bromodomain, particularly the effects of mutation on the acetyl-lysine binding sites. NMR spectroscopy is a powerful method for examining the effects of such a mutation on the conformation of the protein. One can readily obtain information about the global conformation of a mutant protein from the proton (^{1}H) 1D spectrum, by examining the chemical shift dispersion and peak line-width of NMR signals of amide, aromatic and aliphatic protons. Moreover, 2D ^{1}H-^{15}N HSQC spectra reveal details of the effects of a mutation on both local and global conformation of the protein, since every single ^{1}H/^{15}N signal (both the chemical shift and line-shape) in the NMR spectrum is a "reporter" for a particular amino acid residue. Thus, to assess how mutations effect protein stability and the overall protein conformation, the ^{15}N HSQC

spectra of mutated proteins can be compared to that of the wild-type protein bromodomain.

Chemical-shift perturbations due to ligand binding have proven to be a reliable and sensitive probe for the ligand binding site of the protein. This is because the chemical-shift changes of the backbone amide groups are likely to reflect any changes in protein conformation and/or hydrogen bonding due to the peptide/ligand binding. To examine the effects of a mutation on the ligand binding (in this case the ligand is a peptide comprising an acetyl-lysine), peptide titration experiments can be conducted by following the changes of $^{1}H/^{15}N$ signals of the mutant proteins as a function of the peptide concentration. These experiments indicate whether the acetyl-lysine binding site remains the same or changes in the mutants relative to the wild type protein. The effects of the mutation on the peptide binding affinity can also be examined by NMR spectroscopy. If the mutated proteins result in the reduction of the binding affinity, a change of the exchange phenomenon between the free and the ligand-bound signals should be observed in NMR spectrum. If the reduction in binding affinity causes the peptide binding to change from a slow exchange rate to a fast exchange rate, on the NMR time scale, then the peptide binding affinity can be determined from the NMR titration experiment. From these mutation analyses key amino acid residues that are important for binding a peptide comprising the acetyl-lysine can be identified. Such analysis has been exemplified below.

<u>Protein Structure Determination by NMR Spectroscopy</u>

The NMR results from the present invention are summarized by the atomic structure coordinates of the free form of the P/CAF bromodomain (Table 5) and of the P/CAF bromodomain-acetyl-histamine complex (Table 6). The NMR chemical shift assignments of the P/CAF bromodomain are included in the chemical shift table (Table 1) for the ^{1}H-^{15}N HSQC spectrum of P/CAF bromodomain. The unambiguous NOE-derived Inter-proton Distance Restraints are in Table 2, the ambiguous NOE-derived Inter-proton Distance Restraints are in Table 3, and the ^{1}H bonding restraints are disclosed in Table 4.

Backbone and Side-chain Assignments: Sequence-specific backbone assignment can be achieved by using a suite of deuterium-decoupled triple-resonance 3D NMR experiments which include HNCA, HN(CO)CA, HN(CA)CB, HN(COCA)CB, HNCO, and HN(CA)CO experiments [Yamazaki, *et al.*, *J. Am. Chem. Soc.* **116**:11655-11666 (1994)]. The water flip-back scheme is used in these NMR pulse programs to minimize amide signal attenuation from water exchange. Sequential side-chain assignments are typically accomplished from a series of 3D NMR experiments with alternative approaches to confirm the assignments. These experiments include 3D ^{15}N TOCSY-HSQC, HCCH-TOCSY, (H)C(CO)NH-TOCSY, and H(C)(CO)NH-TOCSY [*see* Clore, G. M. & Gronenborn, A. M. *Meth. Enzymol.* **239:**249-363 (1994);Sattler *et al.*, *Prog. in Nuclear Magnetic Resonance Spec.* **4**:93-158 (1999)].

Stereospecific Methyl Groups: Stereospecific assignments of methyl groups of Valine and Leucine residues can be obtained from an analysis of carbon signal multiplet splitting using a fractionally ^{13}C-labeled protein sample, which can be readily prepared using M9 minimal medium containing 10% ^{13}C-/90%^{12}C-glucose mixture [*see* Neri, *et al.*, *Biochemistry* **28**:7510-7516 (1989)].

Dihedral Angle Restraints: Backbone dihedral angle (Φ) constraints can be generated from the $^{3}J_{HNH\alpha}$ coupling constants measured in a HNHA-*J* experiment [*see* Vuister, G. & Bax, A. *J. Am. Chem. Soc.* **115**:7772-7777 (1993)]. Side-chain dihedral angles ($\chi 1$) can be obtained from short mixing time ^{15}N-edited 3D TOCSY-HSQC [*see* Clore, *et al.*, *J, Biomol. NMR* **1**:13-22 (1991)] and 3D HNHB experiments [*see* Matson *et al.*, *J. Biomol. NMR* **3**:239-244 (1993)], which can also provide stereospecific assignments of β methylene protons.

Hydrogen Bonds Restraints: Amide protons that are involved in hydrogen bonds can be identified from an analysis of amide exchange rates measured from a series of 2D $^{1}H/^{15}N$ HSQC spectra recorded after adding $^{2}H_2O$ to the protein sample.

NOE Distance Restraints: Distance restraints are obtained from analysis of ^{15}N, and ^{13}C-edited 3D NOESY data, which can be collected with different mixing times to minimize spin diffusion problems. The nuclear Overhauser effect (NOE)-derived

restraints are categorized as strong (1.8-3 Å), medium (1.8-4 Å) or weak (1.8-5 Å) based on the observed NOE intensities. A recently developed procedure for the iterative automated NOE analysis by using ARIA [*see* Nilges *et al.*, *Prog. NMR Spectroscopy* **32**:107-139 (1998)] can be employed which integrates with X-PLOR for structural calculations. To ensure the success of ARIA/X-PLOR-assisted NOE analysis and structure calculations, the ARIA assigned NOE peaks can be manually confirmed.

Intermolecular NOE Distance Restrains: For the structural determination of a protein/peptide complex, intermolecular NOE distance restraints can be obtained from a ^{13}C-edited (F_1) and ^{15}N, and ^{13}C-filtered (F_3) 3D NOESY data set collected for a sample containing isotope-labeled protein and non-labeled peptide.

Structure Calculations and Refinements: Structures of the protein can be generated using a distance geometry/simulated annealing protocol with the X-PLOR program [*see* Nilges,*et al.*, *FEBS Lett.* **229**:317-324 (1988); Kuszewski, *et al.*, *J. Biolmol. NMR* **2**:33-56 (1992); Brünger, A. T. *X-PLOR Version 3.1: A system for X-Ray crystallography and NMR* (Yale University Press, New Haven, CT, 1993)]. The structure calculations can employ inter-proton distance restraints obtained from ^{15}N- and ^{13}C-resolved NOESY spectra. The initial low-resolution structures can be used to facilitate NOE assignments, and help identify hydrogen bonding partners for slowly exchanging amide protons. The experimental restraints of dihedral angles and hydrogen bonds can be included in the distance restraints for structure refinements.

Protein-Structure Based Design of Agonists and Antagonists of the Bromodomain-Acetyl-Lysine Binding Complex

Once the three-dimensional structure of the Bromodomain and the Bromodomain-acetyl-lysine binding complex are determined, a potential drug or agent (antagonist or agonist) can be examined through the use of computer modeling using a docking program such as GRAM, DOCK, or AUTODOCK [Dunbrack *et al.*, 1997, *supra*]. This procedure can include computer fitting of potential agents to the bromodomain, for example, to ascertain how well the shape and the chemical structure of the potential ligand will complement or interfere with the interaction between the bromodomain and

the acetyl-lysine [Bugg *et al.*, *Scientific American*, **Dec.**:92-98 (1993); West *et al.*, *TIPS*, **16**:67-74 (1995)]. Computer programs can also be employed to estimate the attraction, repulsion, and steric hindrance of the agent to the dimer-dimer binding site, for example. Generally the tighter the fit (*e.g.*, the lower the steric hindrance, and/or the greater the attractive force) the more potent the potential drug will be since these properties are consistent with a tighter binding constant. Furthermore, the more specificity in the design of a potential drug the more likely that the drug will not interfere with related proteins. This will minimize potential side-effects due to unwanted interactions with other proteins.

Initially a potential drug could be obtained by screening a random peptide library produced by recombinant bacteriophage for example, [Scott and Smith, *Science*, **249**:386-390 (1990); Cwirla *et al.*, *Proc. Natl. Acad. Sci.*, **87**:6378-6382 (1990); Devlin *et al.*, *Science*, **249**:404-406 (1990)] or a chemical library. An agent selected in this manner could be then be systematically modified by computer modeling programs until one or more promising potential drugs are identified. Such analysis has been shown to be effective in the development of HIV protease inhibitors [Lam *et al.*, *Science* **263**:380-384 (1994); Wlodawer *et al.*, *Ann. Rev. Biochem.* **62**:543-585 (1993); Appelt, *Perspectives in Drug Discovery and Design* **1**:23-48 (1993); Erickson, *Perspectives in Drug Discovery and Design* **1**:109-128 (1993)].

Such computer modeling allows the selection of a finite number of rational chemical modifications, as opposed to the countless number of essentially random chemical modifications that could be made, any one of which might lead to a useful drug. Each chemical modification requires additional chemical steps, which while being reasonable for the synthesis of a finite number of compounds, quickly becomes overwhelming if all possible modifications needed to be synthesized. Thus, through the use of the three-dimensional structural analysis disclosed herein and computer modeling, a large number of these compounds can be rapidly screened on the computer monitor screen, and a few likely candidates can be determined without the laborious synthesis of untold numbers of compounds.

Once a potential drug (agonist or antagonist) is identified it can be either selected from a library of chemicals as are commercially available from most large chemical companies including Merck, GlaxoWelcome, Bristol Meyers Squib, Monsanto/Searle, Eli Lilly, Novartis and Pharmacia UpJohn, or alternatively the potential drug may be synthesized *de novo*. As mentioned above, the *de novo* synthesis of one or even a relatively small group of specific compounds is reasonable in the art of drug design.

The potential drug can then be tested in any standard binding assay (including in high throughput binding assays) for its ability to bind to the ZA loop of a bromodomain. Alternatively the potential drug can be tested for its ability to modulate the binding of a bromodomain to acetylated histamine, for example. When a suitable potential drug is identified, a second NMR structural analysis can optionally be performed on the binding complex formed between the bromodomain-acetyl-lysine binding complex, or the bromodomain alone and the potential drug. Computer programs that can be used to aid in solving such three-dimensional structures include QUANTA, CHARMM, INSIGHT, SYBYL, MACROMODE, and ICM, MOLMOL, RASMOL, AND GRASP [Kraulis, *J. Appl Crystallogr.* **24**:946-950 (1991)]. Most if not all of these programs and others as well can be also obtained from the WorldWideWeb through the internet.

Using the approach described herein and equipped with the structural analysis disclosed herein, the three-dimensional structures of other bromodomain-acetyl-lysine binding complexes can more readily be obtained and analyzed. Such analysis will, in turn, allow corresponding drug screening methodology to be performed using the three-dimensional structures of such related complexes.

For all of the drug screening assays described herein further refinements to the structure of the drug will generally be necessary and can be made by the successive iterations of any and/or all of the steps provided by the particular drug screening assay, including further structural analysis by NMR, for example.

Phage libraries for Drug Screening.

Phage libraries have been constructed which when infected into host *E. coli* produce random peptide sequences of approximately 10 to 15 amino acids [Parmley and Smith,

Gene **73**:305-318 (1988), Scott and Smith, Science **249**:386-249 (1990)]. Specifically, the phage library can be mixed in low dilutions with permissive *E. coli* in low melting point LB agar which is then poured on top of LB agar plates. After incubating the plates at 37°C for a period of time, small clear plaques in a lawn of *E. coli* will form which represents active phage growth and lysis of the *E. coli*. A representative of these phages can be absorbed to nylon filters by placing dry filters onto the agar plates. The filters can be marked for orientation, removed, and placed in washing solutions to block any remaining absorbent sites. The filters can then be placed in a solution containing, for example, a radioactive bromodomain. After a specified incubation period, the filters can be thoroughly washed and developed for autoradiography. Plaques containing the phage that bind to the radioactive bromodomain can then be identified. These phages can be further cloned and then retested for their ability to bind to the bromodomain as before. Once the phage has been purified, the binding sequence contained within the phage can be determined by standard DNA sequencing techniques. Once the DNA sequence is known, synthetic peptides can be generated which are encoded by these sequences. These peptides can be tested, for example, for their ability to modulate the affinity of the bromodomain for its binding partner (*e.g.*, a protein comprising an acetyl-lysine or a fragment of that protein).

The effective peptide(s) can be synthesized in large quantities for use in *in vivo* models and eventually in humans to treat certain tumors. It should be emphasized that synthetic peptide production is relatively non-labor intensive, easily manufactured, quality controlled and thus, large quantities of the desired product can be produced quite cheaply. Similar combinations of mass produced synthetic peptides have been used with great success [Patarroyo, *Vaccine,* **10:**175-178 (1990)].

Drug Screening Assays

The drug screening assays of the present invention may use any of a number of means for determining the interaction between an agent or drug and a peptide comprising an acetyl-lysine and/or a bromodomain. Thus, standard high throughput drug screening procedures can be employed using a library of low molecular weight compounds, for

example that can be screened to identify a binding partner for the bromodoamin. Any such chemical library can be used including those discussed above.

In a particular assay, a bromodomain is placed on or coated onto a solid support. Methods for placing the peptides or proteins on the solid support are well known in the art and include such things as linking biotin to the protein and linking avidin to the solid support. An agent is allowed to equilibrate with the bromodomain to test for binding. Generally, the solid support is washed and agents that are retained are selected as potential drugs. Alternatively, a peptide comprising an acetyl-lysine is placed on or coated onto a solid support. In a particular embodiment of this type, the peptide comprises the amino acid sequence of SEQ ID NO:4.

The agent may be labeled. For example, in one embodiment radiolabeled agents are used to measure the binding of the agent. In another embodiment the agents have fluorescent markers. In yet another embodiment, a Biocore chip (Pharmacia) coated with the bromodomain is used, for example and the change in surface conductivity can be measured.

In addition, since a number of proteins have been identified that contain bromodomains, and the binding partners of many of these proteins are known, the fact that the bromodomain specifically binds to an acetylated lysine as disclosed herein allows the identification and preparation of a number of potential modulators of the bromodomain-acetyl-lysine binding complex based on the amino acid sequences of the binding partners to the proteins. Such potential modulators include : ISYGR-*AcK*-KRRQRR (SEQ ID NO:4), ARKSTGG-A*cK*-APRKQL (SEQ ID NO:5) and QSTSRHK-*AcK*-LMFKTE (SEQ ID NO:6) which bind to the P/CAF bromodomain as shown in the Example, below. Such peptides also can be used, for example, as a starting point for the design of an inhibitor of the bromodomain-acetyl-lysine binding complex.

Alternatively, a drug can be specifically designed to bind to the ZA loop of a bromodomain for example, such as the P/CAF bromodomain, and be assayed through NMR based methodology [Shuker *et al.*, *Science* **274**:1531-1534 (1996) hereby

incorporated by reference in its entirety.] In a particular embodiment, analogs of the binding partner of the bromodomain can be used in this analysis. One such peptide has the amino acid sequence of SEQ ID NO:4. In another embodiment of this type, the peptide has the amino acid sequence of SEQ ID NO:5. In another such embodiment of this type, the peptide has the amino acid sequence of SEQ ID NO:6.

The assay begins with contacting a compound with a ^{15}N-labeled bromodomain. Binding of the compound with the ZA loop of the bromodomain can be determined by monitoring the ^{15}N- or ^{1}H-amide chemical shift changes in two dimensional ^{15}N-heteronuclear single-quantum correlation (^{15}N-HSQC) spectra upon the addition of the compound to the ^{15}N-labeled bromodomain. Since these spectra can be rapidly obtained, it is feasible to screen a large number of compounds [Shuker *et al.*, *Science* **274**:1531-1534 (1996)]. A compound is identified as a potential ligand if it binds to the ZA loop of the bromodomain. In a further embodiment, the potential ligand can then be used as a model structure, and analogs to the compound can be obtained (e.g, from the vast chemical libraries commercially available, or alternatively through *de novo* synthesis). The analogs are then screened for their ability to bind the ZA loop of the bromodomain thus to obtain a ligand. An analog of the potential ligand is chosen as a ligand when it binds to the ZA loop of the bromodomain with a higher binding affinity than the potential ligand. In a preferred embodiment of this type the analogs are screened by monitoring the ^{15}N- or ^{1}H-amide chemical shift changes in two dimensional ^{15}N-heteronuclear single-quantum correlation (^{15}N-HSQC) spectra upon the addition of the analog to the ^{15}N-labeled bromodomain as described above.

In another further embodiment, compounds are screened for binding to two nearby sites on the bromodomain. In this case, a compound that binds a first site of the bromodomain does not bind a second nearby site. Binding to the second site can be determined by monitoring changes in a different set of amide chemical shifts in either the original screen or a second screen conducted in the presence of a ligand (or potential ligand) for the first site. From an analysis of the chemical shift changes the approximate location of a potential ligand for the second site is identified. Optimization of the second ligand for binding to the site is then carried out by screening structurally related compounds (*e.g.*, analogs as described above). When

ligands for the first site and the second site are identified, their location and orientation in the ternary complex can be determined experimentally either by NMR spectroscopy or X-ray crystallography. On the basis of this structural information, a linked compound is synthesized in which the ligand for the first site and the ligand for the second site are linked. In a preferred embodiment of this type the two ligands are covalently linked. This linked compound is tested to determine if it has a higher binding affinity for the bromodomain than either of the two individual ligands. A linked compound is selected as a ligand when it has a higher binding affinity for the bromodomain than either of the two ligands. In a preferred embodiment the affinity of the linked compound with the bromodomain is determined monitoring the ^{15}N- or ^{1}H-amide chemical shift changes in two dimensional ^{15}N-heteronuclear single-quantum correlation (^{15}N-HSQC) spectra upon the addition of the linked compound to the ^{15}N-labeled bromodomain as described above.

A larger linked compound can be constructed in an analogous manner, *e.g.*, linking three ligands which bind to three nearby sites on the bromodomain to form a multilinked compound that has an even higher affinity for the bromodomain than the linked compound.

Identification of New Bromodomains

By disclosing that protein bound acetyl-lysine is a binding partner for bromodomains, the present invention provides a method of identifying novel proteins that contain bromodomains. In short, a protein fragment or analog thereof comprising an acetyl-lysine can be used as bait to identify a binding partner that comprises a bromodomain. Any one of a number of procedures can be carried out to identify such a binding partner. One such assay comprises passing a cell extract over the bait peptide which is attached to a solid support. After washing the solid support to remove any non-specific binders, the bromodomain containing protein can be eluted from the solid support with an appropriate eluant. In a particular embodiment, the free bait peptide can be used in the elution. Other methodology includes the use of a yeast two-hybrid system, a GST pull down assay, ELISA, immunometric assays, and a modification of the CORT procedure of Schlessinger *et al.*, (US Patent No. 5,858,686, Issued on

January 12, 1999 which is hereby incorporated by reference in its entirety) for use with the bromodomain-acetyl-lysine binding complex.

Labels:

Suitable labels include enzymes, fluorophores (*e.g.*, fluorescein isothiocyanate (FITC), phycoerythrin (PE), Texas red (TR), rhodamine, free or chelated lanthanide series salts, especially Eu^{3+}, to name a few fluorophores), chromophores, radioisotopes, chelating agents, dyes, colloidal gold, latex particles, ligands (*e.g.*, biotin), and chemiluminescent agents. When a control marker is employed, the same or different labels may be used for the test and control marker gene.

In the instance where a radioactive label, such as the isotopes ^{3}H, ^{14}C, ^{32}P, ^{35}S, ^{36}Cl, ^{51}Cr, ^{57}Co, ^{58}Co, ^{59}Fe, ^{90}Y, ^{125}I, ^{131}I, and ^{186}Re are used, known currently available counting procedures may be utilized. In the instance where the label is an enzyme, detection may be accomplished by any of the presently utilized colorimetric, spectrophotometric, fluorospectrophotometric, amperometric or gasometric techniques known in the art.

Direct labels are one example of labels which can be used according to the present invention. A direct label has been defined as an entity, which in its natural state, is readily visible, either to the naked eye, or with the aid of an optical filter and/or applied stimulation, e.g. U.V. light to promote fluorescence. Among examples of colored labels, which can be used according to the present invention, include metallic sol particles, for example, gold sol particles such as those described by Leuvering (U.S. Patent 4,313,734); dye sole particles such as described by Gribnau *et al.* (U.S. Patent 4,373,932 and May *et al.* (WO 88/08534); dyed latex such as described by May, *supra*, Snyder (EP-A 0 280 559 and 0 281 327); or dyes encapsulated in liposomes as described by Campbell et al. (U.S. Patent 4,703,017). Other direct labels include a radionucleotide, a fluorescent moiety or a luminescent moiety. In addition to these direct labeling devices, indirect labels comprising enzymes can also be used according to the present invention. Various types of enzyme linked immunoassays are well known in the art, for example, alkaline phosphatase and horseradish peroxidase,

lysozyme, glucose-6-phosphate dehydrogenase, lactate dehydrogenase, urease, these and others have been discussed in detail by Eva Engvall in Enzyme Immunoassay ELISA and EMIT in *Methods in Enzymology*, **70:**419-439 (1980) and in U.S. Patent 4,857,453.

Suitable enzymes include, but are not limited to, alkaline phosphatase, β-galactosidase, green fluorescent protein and its derivatives, luciferase, and horseradish peroxidase.

Other labels for use in the invention include magnetic beads or magnetic resonance imaging labels.

Antibodies to Portions of the Bromodomain that Interact with Acetyl-Lysine

According to the present invention, the bromodomains, and more particularly the ZA loops of the bromodomains and fragments thereof can be produced by a recombinant source, or through chemical synthesis, or through the modification of these peptides and fragments; and derivatives or analogs thereof, including fusion proteins, may be used as an immunogen to generate antibodies that specifically interfere with the formation of the bromodomain-acetyl-lysine binding complex. Similarly, antibodies can be raised against peptides that comprise one or more acetyl-lysine residues which also interfere with the formation of the bromodomain-acetyl-lysine binding complex. Such antibodies include but are not limited to polyclonal, monoclonal, chimeric, single chain, Fab fragments, and a Fab expression library.

Various procedures known in the art may be used for the production of the polyclonal antibodies. For the production of antibody, various host animals can be immunized by injection with the peptide having the amino acid sequence of SEQ ID NO:3, for example, or a derivative (*e.g.*, or fusion protein) thereof, including but not limited to rabbits, mice, rats, sheep, goats, etc. In one embodiment, the peptide can be conjugated to an immunogenic carrier, *e.g.*, bovine serum albumin (BSA) or keyhole limpet hemocyanin (KLH). Various adjuvants may be used to increase the immunological response, depending on the host species, including but not limited to Freund's (complete and incomplete), mineral gels such as aluminum hydroxide, surface

active substances such as lysolecithin, pluronic polyols, polyanions, peptides, oil emulsions, keyhole limpet hemocyanins, dinitrophenol, and potentially useful human adjuvants such as BCG (*bacille Calmette-Guerin*) and *Corynebacterium parvum*.

For preparation of monoclonal antibodies directed toward the peptides or protein fragments of the present invention, or analog, or derivative thereof, any technique that provides for the production of antibody molecules by continuous cell lines in culture may be used. These include but are not limited to the hybridoma technique originally developed by Kohler and Milstein [*Nature,* **256**:495-497 (1975)], as well as the trioma technique, the human B-cell hybridoma technique [Kozbor *et al., Immunology Today,* **4**:72 (1983); Cote *et al., Proc. Natl. Acad. Sci. U.S.A.,* **80**:2026-2030 (1983)], and the EBV-hybridoma technique to produce human monoclonal antibodies [Cole *et al.,* in *Monoclonal Antibodies and Cancer Therapy*, Alan R. Liss, Inc., pp. 77-96 (1985)]. In an additional embodiment of the invention, monoclonal antibodies can be produced in germ-free animals utilizing technology described in PCT/US90/02545. In fact, according to the invention, techniques developed for the production of "chimeric antibodies" [Morrison *et al., J. Bacteriol.*, **159**:870 (1984); Neuberger *et al., Nature,* **312**:604-608 (1984); Takeda *et al.*, *Nature,* **314**:452-454 (1985)] by splicing the genes from a mouse antibody molecule specific for the peptide having the amino acid sequence of SEQ ID NO:3, for example, together with genes from a human antibody molecule of appropriate biological activity can be used; such antibodies are within the scope of this invention. Such human or humanized chimeric antibodies are preferred for use in therapy of human diseases or disorders (described *infra*), since the human or humanized antibodies are much less likely than xenogenic antibodies to induce an immune response, in particular an allergic response, themselves.

According to the invention, techniques described for the production of single chain antibodies [U.S. Patent Nos. 5,476,786 and 5,132,405 to Huston; U.S. Patent 4,946,778] can be adapted to produce specific single chain antibodies. An additional embodiment of the invention utilizes the techniques described for the construction of Fab expression libraries [Huse *et al., Science,* **246**:1275-1281 (1989)] to allow rapid and easy identification of monoclonal Fab fragments with the desired specificity.

Antibody fragments which contain the idiotype of the antibody molecule can be generated by known techniques. For example, such fragments include but are not limited to: the $F(ab')_2$ fragment which can be produced by pepsin digestion of the antibody molecule; the Fab' fragments which can be generated by reducing the disulfide bridges of the $F(ab')_2$ fragment, and the Fab fragments which can be generated by treating the antibody molecule with papain and a reducing agent.

In the production of antibodies, screening for the desired antibody can be accomplished by techniques known in the art, *e.g.*, radioimmunoassay, ELISA (enzyme-linked immunosorbant assay), "sandwich" immunoassays, immunoradiometric assays, gel diffusion precipitin reactions, immunodiffusion assays, *in situ* immunoassays (using colloidal gold, enzyme or radioisotope labels, for example), western blots, precipitation reactions, agglutination assays (*e.g.*, gel agglutination assays, hemagglutination assays), complement fixation assays, immunofluorescence assays, protein A assays, and immunoelectrophoresis assays, etc. In one embodiment, antibody binding is detected by detecting a label on the primary antibody. In another embodiment, the primary antibody is detected by detecting binding of a secondary antibody or reagent to the primary antibody. In a further embodiment, the secondary antibody is labeled. Many means are known in the art for detecting binding in an immunoassay and are within the scope of the present invention. For example, to select antibodies which recognize a specific epitope of a ZA loop of a bromodomain, for example, one may assay generated hybridomas for a product which binds to a bromodomain fragment containing such an epitope and choose those which do not cross-react with bromodomain fragments that do not include that epitope.

In a specific embodiment, antibodies that interfere with the formation of the bromodomain-acetyl-lysine complex can be generated. Such antibodies can be tested using the assays described and could potentially be used in anti-cancer therapies.

Administration

According to the invention, the component or components of a therapeutic composition, *e.g.*, an agent of the invention that interferes with the bromodomain-

acetyl-lysine binding complex such as the peptide having the amino acid sequence of SEQ ID NOs:4, 5, or 6 and a pharmaceutically acceptable carrier, may be introduced parenterally, transmucosally, *e.g.*, orally, nasally, or rectally, or transdermally. Preferably, administration is parenteral, *e.g.*, via intravenous injection, and also including, but is not limited to, intra-arteriole, intramuscular, intradermal, subcutaneous, intraperitoneal, intraventricular, and intracranial administration.

In a preferred aspect, the agent of the present invention can cross cellular and nuclear membranes, which would allow for intravenous or oral administration. Strategies are available for such crossing, including but not limited to, increasing the hydrophobic nature of a molecule; introducing the molecule as a conjugate to a carrier, such as a ligand to a specific receptor, targeted to a receptor; and the like.

The present invention also provides for conjugating targeting molecules to such an agent. "Targeting molecule" as used herein shall mean a molecule which, when administered *in vivo*, localizes to desired location(s). In various embodiments, the targeting molecule can be a peptide or protein, antibody, lectin, carbohydrate, or steroid. In one embodiment, the targeting molecule is a peptide ligand of a receptor on the target cell. In a specific embodiment, the targeting molecule is an antibody. Preferably, the targeting molecule is a monoclonal antibody. In one embodiment, to facilitate crosslinking the antibody can be reduced to two heavy and light chain heterodimers, or the $F(ab')_2$ fragment can be reduced, and crosslinked to the agent via the reduced sulfhydryl. Antibodies for use as targeting molecule are specific for a cell surface antigen.

In another embodiment, the therapeutic compound can be delivered in a vesicle, in particular a liposome [*see* Langer, *Science,* **249**:1527-1533 (1990); Treat *et al.*, in *Liposomes in the Therapy of Infectious Disease and Cancer*, Lopez-Berestein and Fidler (eds.), Liss: New York, pp. 353-365 (1989); Lopez-Berestein, *ibid.*, pp. 317-327; see generally *ibid.*].

In yet another embodiment, the therapeutic compound can be delivered in a controlled release system. For example, the agent may be administered using intravenous

infusion, an implantable osmotic pump, a transdermal patch, liposomes, or other modes of administration. In one embodiment, a pump may be used [*see* Langer, *supra*; Sefton, *CRC Crit. Ref. Biomed. Eng.*, **14**:201 (1987); Buchwald *et al.*, *Surgery,* **88**:507 (1980); Saudek *et al.*, *N. Engl. J. Med.*, **321**:574 (1989)]. In another embodiment, polymeric materials can be used [*see Medical Applications of Controlled Release*, Langer and Wise (eds.), CRC Press: Boca Raton, Florida (1974); *Controlled Drug Bioavailability, Drug Product Design and Performance*, Smolen and Ball (eds.), Wiley: New York (1984); Ranger and Peppas, *J. Macromol. Sci. Rev. Macromol. Chem.*, **23**:61 (1983); see also Levy *et al.*, *Science*, **228**:190 (1985); During *et al.*, *Ann. Neurol.*, **25**:351 (1989); Howard *et al.*, *J. Neurosurg.*, **71**:105 (1989)]. In yet another embodiment, a controlled release system can be placed in proximity of the therapeutic target, *i.e.*, the bone marrow, thus requiring only a fraction of the systemic dose [*see, e.g.*, Goodson, in *Medical Applications of Controlled Release*, *supra*, vol. 2, pp. 115-138 (1984)]. Other controlled release systems are discussed in the review by Langer [*Science,* **249**:1527-1533 (1990)].

Pharmaceutical Compositions. In yet another aspect of the present invention, provided are pharmaceutical compositions of the above. Such pharmaceutical compositions may be for administration for injection, or for oral, pulmonary, nasal or other forms of administration. In general, comprehended by the invention are pharmaceutical compositions comprising effective amounts of a low molecular weight component or components, or derivative products, of the invention together with pharmaceutically acceptable diluents, preservatives, solubilizers, emulsifiers, adjuvants and/or carriers. Such compositions include diluents of various buffer content (*e.g.*, Tris-HCl, acetate, phosphate), pH and ionic strength; additives such as detergents and solubilizing agents (*e.g.*, Tween 80, Polysorbate 80), anti-oxidants (*e.g.*, ascorbic acid, sodium metabisulfite), preservatives (*e.g.*, Thimersol, benzyl alcohol) and bulking substances (*e.g.*, lactose, mannitol); incorporation of the material into particulate preparations of polymeric compounds such as polylactic acid, polyglycolic acid, etc. or into liposomes. Hylauronic acid may also be used. Such compositions may influence the physical state, stability, rate of *in vivo* release, and rate of *in vivo* clearance of the present proteins and derivatives. *See, e.g.*, Remington's Pharmaceutical Sciences, 18th Ed. [1990, Mack Publishing Co., Easton, PA 18042] pages 1435-1712 which are herein

incorporated by reference. The compositions may be prepared in liquid form, or may be in dried powder, such as lyophilized form.

Oral Delivery. Contemplated for use herein are oral solid dosage forms, which are described generally in Remington's Pharmaceutical Sciences, 18th Ed.1990 (Mack Publishing Co. Easton PA 18042) at Chapter 89, which is herein incorporated by reference. Solid dosage forms include tablets, capsules, pills, troches or lozenges, cachets or pellets. Also, liposomal or proteinoid encapsulation may be used to formulate the present compositions (as, for example, proteinoid microspheres reported in U.S. Patent No. 4,925,673). Liposomal encapsulation may be used and the liposomes may be derivatized with various polymers (*e.g.*, U.S. Patent No. 5,013,556). A description of possible solid dosage forms for the therapeutic is given by Marshall, K. In: *Modern Pharmaceutics* Edited by G.S. Banker and C.T. Rhodes Chapter 10, 1979, herein incorporated by reference. In general, the formulation will include an agent of the present invention (or chemically modified forms thereof) and inert ingredients which allow for protection against the stomach environment, and release of the biologically active material in the intestine.

Also specifically contemplated are oral dosage forms of the above derivatized component or components. The component or components may be chemically modified so that oral delivery of the derivative is efficacious. Generally, the chemical modification contemplated is the attachment of at least one moiety to the component molecule itself, where said moiety permits (a) inhibition of proteolysis; and (b) uptake into the blood stream from the stomach or intestine. Also desired is the increase in overall stability of the component or components and increase in circulation time in the body. An example of such a moiety is polyethylene glycol.

For the component (or derivative) the location of release may be the stomach, the small intestine (the duodenum, the jejunum, or the ileum), or the large intestine. One skilled in the art has available formulations which will not dissolve in the stomach, yet will release the material in the duodenum or elsewhere in the intestine. Preferably, the release will avoid the deleterious effects of the stomach environment, either by

protection of the protein (or derivative) or by release of the biologically active material beyond the stomach environment, such as in the intestine.

The therapeutic can be included in the formulation as fine multi-particulates in the form of granules or pellets of particle size about 1 mm. The formulation of the material for capsule administration could also be as a powder, lightly compressed plugs or even as tablets. The therapeutic could be prepared by compression.

One may dilute or increase the volume of the therapeutic with an inert material. These diluents could include carbohydrates, especially mannitol, a-lactose, anhydrous lactose, cellulose, sucrose, modified dextrans and starch. Certain inorganic salts may be also be used as fillers including calcium triphosphate, magnesium carbonate and sodium chloride. Some commercially available diluents are Fast-Flo, Emdex, STA-Rx 1500, Emcompress and Avicell.

Disintegrants may be included in the formulation of the therapeutic into a solid dosage form. Materials used as disintegrates include but are not limited to starch, including the commercial disintegrant based on starch, Explotab. Binders also may be used to hold the therapeutic agent together to form a hard tablet and include materials from natural products such as acacia, tragacanth, starch and gelatin.

An anti-frictional agent may be included in the formulation of the therapeutic to prevent sticking during the formulation process. Lubricants may be used as a layer between the therapeutic and the die wall. Glidants that might improve the flow properties of the drug during formulation and to aid rearrangement during compression also might be added. The glidants may include starch, talc, pyrogenic silica and hydrated silicoaluminate.

In addition, to aid dissolution of the therapeutic into the aqueous environment a surfactant might be added as a wetting agent. Additives which potentially enhance uptake of the protein (or derivative) are for instance the fatty acids oleic acid, linoleic acid and linolenic acid.

Nasal Delivery. Nasal delivery of an agent of the present invention (or derivative) is also contemplated. Nasal delivery allows the passage of a peptide, for example, to the blood stream directly after administering the therapeutic product to the nose, without the necessity for deposition of the product in the lung. Formulations for nasal delivery include those with dextran or cyclodextran.

Transdermal administration. Various and numerous methods are known in the art for transdermal administration of a drug, *e.g.*, via a transdermal patch. Transdermal patches are described in for example, U.S. Patent No. 5,407,713, issued April 18, 1995 to Rolando *et al.*; U.S. Patent No. 5,352,456, issued October 4, 1004 to Fallon *et al.*; U.S. Patent No. 5,332,213 issued August 9, 1994 to D'Angelo *et al.*; U.S. Patent No. 5,336,168, issued August 9, 1994 to Sibalis; U.S. Patent No. 5,290,561, issued March 1, 1994 to Farhadieh *et al.*; U.S. Patent No. 5,254,346, issued October 19, 1993 to Tucker *et al.*; U.S. Patent No. 5,164,189, issued November 17, 1992 to Berger *et al.*; U.S. Patent No. 5,163,899, issued November 17, 1992 to Sibalis; U.S. Patent Nos. 5,088,977 and 5,087,240, both issued February 18, 1992 to Sibalis; U.S. Patent No. 5,008,110, issued April 16, 1991 to Benecke *et al.*; and U.S. Patent No. 4,921,475, issued May 1, 1990 to Sibalis, the disclosure of each of which is incorporated herein by reference in its entirety.

It can be readily appreciated that a transdermal route of administration may be enhanced by use of a dermal penetration enhancer, *e.g.*, such as enhancers described in U.S. Patent No. 5,164,189 (*supra*), U.S. Patent No. 5,008,110 (*supra*), and U.S. Patent No. 4,879,119, issued November 7, 1989 to Aruga *et al.*, the disclosure of each of which is incorporated herein by reference in its entirety.

Pulmonary Delivery. Also contemplated herein is pulmonary delivery of the pharmaceutical compositions of the present invention. A pharmaceutical composition of the present invention is delivered to the lungs of a mammal while inhaling and traverses across the lung epithelial lining to the blood stream. Other reports of this include Adjei *et al.* [*Pharmaceutical Research*, **7**:565-569 (1990); Adjei et al., *International Journal of Pharmaceutics*, **63**:135-144 (1990) (leuprolide acetate); Braquet *et al., Journal of Cardiovascular Pharmacology*, **13(suppl. 5):**143-146 (1989)

(endothelin-1); Hubbard *et al., Annals of Internal Medicine*, **Vol. III**, pp. 206-212 (1989) (α1-antitrypsin); Smith *et al., J. Clin. Invest.*, **84**:1145-1146 (1989) (α-1-proteinase); Oswein *et al.*, "Aerosolization of Proteins", *Proceedings of Symposium on Respiratory Drug Delivery II*, Keystone, Colorado, March, (1990) (recombinant human growth hormone); Debs et al., *J. Immunol.*, **140**:3482-3488 (1988) (interferon-γ and tumor necrosis factor alpha); Platz *et al.*, U.S. Patent No. 5,284,656 (granulocyte colony stimulating factor)]. A method and composition for pulmonary delivery of drugs for systemic effect is described in U.S. Patent No. 5,451,569, issued September 19, 1995 to Wong *et al.*

A subject in whom administration of an agent of the present invention is an effective therapeutic regiment for cancer, for example, is preferably a human, but can be any animal. Thus, as can be readily appreciated by one of ordinary skill in the art, the methods and pharmaceutical compositions of the present invention are particularly suited to administration to any animal, *e.g.*, for veterinary medical use, particularly for a mammal, and including, but by no means limited to, domestic animals, such as feline or canine subjects, farm animals, including bovine, equine, caprine, ovine, and porcine subjects, wild animals (whether in the wild or in a zoological garden), research animals, such as mice, rats, rabbits, goats, sheep, pigs, dogs, cats, avian species, such as chickens, turkeys, and songbirds.

The present invention may be better understood by reference to the following non-limiting Example, which is provided as exemplary of the invention. The following example is presented in order to more fully illustrate the preferred embodiments of the invention. It should in no way be construed, however, as limiting the broad scope of the invention.

EXAMPLE

STRUCTURE AND LIGAND OF A HISTONE ACETYLTRANSFERASE BROMODOMAIN

Introduction

The bromodomain is a protein motif comprising approximately 110 amino acids that is found in practically all nuclear histone acetyltransferases (HATs) [Jeanmougin *et al.*, Trends in Biochemical *Sciences*, **22:**151-153 (1997)]. However, despite the seemingly requisite occurrence of this motif in HATs, their role in these enzymes is unknown. Indeed, although this motif has also been identified in other chromatin proteins, heretofore not even one binding partner for a bromodomain had been identified.

Materials and Methods

Sample preparation: The bromodomain of P/CAF (residues 719-832 of SEQ ID NO:2) was subcloned into the pET14b expression vector (Novagen) and expressed in *Escherichia coli* BL21(DE3) cells. Uniformly ^{15}N- and $^{15}N/^{13}C$-labelled proteins were prepared by growing bacteria in a minimal medium containing $^{15}NH_4Cl$ with or without $^{13}C_6$-glucose. A uniformly $^{15}N/^{13}C$-labelled and fractionally deuterated protein sample was prepared by growing the cells in 75% ^2H_2O. The bromodomain was purified by affinity chromatography on a nickel-IDA column (Invitrogen) followed by the removal of poly-His tag by thrombin cleavage. The final purification of the protein was achieved by size-exclusion chromatography. The acetyl-lysine-containing peptides were prepared on a MilliGen 9050 peptide synthesizer (Perkin Elmer) using Fmoc/HBTU chemistry. Acetyl-lysine was incorporated using the reagent Fmoc-Ac-Lys with HBTU/DIPEA activation. NMR samples contained approximately 1 mM protein in 100mM phosphate buffer of pH 6.5 and 5mM perdeuterated DTT and 0.5mM EDTA in $H_2O/^2H_2O$ (9/1) or ^2H_2O.

NMR spectroscopy: All NMR spectra were acquired at 30°C on a Bruker DRX600 or DRX500 spectrometer. The backbone assignments of the ^1H, ^{13}C, and ^{15}N resonances were achieved using deuterium-decoupled triple-resonance experiments of HNCACB and HN(CO)CACB [Yamazaki *et al.*, *J. Am. Chem. Soc.* **116**:11655-11666 (1994)] recorded using the uniformly $^{15}N/^{13}C$-labeled and fractionally deuterated protein. The

side-chain atoms were assigned from 3D HCCH-TOCSY [Clore and Gronenborn, *Meth. Enzymol.* **239**:249-363 (1994)] and (H)C(CO)NH-TOCSY [Logan *et al.*, *J. Biolmol. NMR* **3**:225-231 (1993)] data collected on the uniformly $^{15}N/^{13}C$-labeled protein. Stereospecific assignments of methyl groups of the Val and Leu residues were obtained using a fractionally ^{13}C-labeled sample [Neri *et al.*, *Biochemistry* **28**:7510-7516 (1989)]. The NOE-derived distance restraints were obtained from ^{15}N- or ^{13}C-edited 3D NOESY spectra. ϕ-angle restraints were determined based on the $^{3}J_{HN,H\alpha}$ coupling constants measured in a 3D HNHA spectrum [Clore and Gronenborn, *Meth. Enzymol.* **239**:249-363 (1994)]. Slowly exchanging amide protons were identified from a series of 2D ^{15}N-HSQC spectra recorded after the H_2O buffer was changed to a $^{2}H_2O$ buffer. The intermolecular NOEs used in defining the structure of the bromodomain/Ac-histamine complex were detected in ^{13}C-edited (F_1), $^{13}C/^{15}N$-filtered (F_3) 3D NOESY spectrum [Clore and Gronenborn, *Meth. Enzymol.* **239**:249-363 (1994)]. All NMR spectra were processed with the NMRPipe/NMRDraw programs and analyzed using NMRView [Johnson and Blevins, *J. Biomol., NMR* **4**:603-614 (1994)].

Structure calculations: Structures of the bromodomain were calculated with a distance geometry/simulated annealing protocol using the X-PLOR program [Brunger, A. *X-PLOR Version 3.1*: *A system for X-Ray crystallography and NMR*, Yale University Press, New Haven, CT, (1993)]. A total of 1324 manually assigned NOE-derived distance restraints were obtained from the ^{15}N- and ^{13}C-edited NOE spectra. Further analysis of the NOE spectra was carried out by the iterative automated assignment procedure using ARIA [Nilges and O'Donoghue, *Prog. NMR Spectroscopy* **32**:107-139 (1998)], which integrates with X-PLOR for structure calculations. A total of 1519 unambiguous and 590 ambiguous distance restraints were identified from the NOE data by ARIA, many of which were checked and confirmed manually. The ARIA-assigned distance restraints were in agreement with the structures calculated using only the manually assigned NOE distance restraints, 28 hydrogen-bond distance restraints for 14 hydrogen bonds, and 54 ϕ-angle restraints. The final structure calculations employed a total of 3515 NMR experimental restraints obtained from the manual and the ARIA-assisted assignments, 2843 of which were unambiguously assigned NOE-derived distance restraints that comprise of 1077 intra-residue, 621

sequential, 550 medium-range, and 595 long-range NOEs. For the ensemble of the final 30 structures, no distance and torsional angle restraints were violated by more than 0.3Å and 5°, respectively. The total, distance violation, and dihedral violation energies were 178.7 ± 2.4 kcal mol^{-1}, 41.6 ± 0.9 kcal mol^{-1}, and 0.50 ± 0.06 kcal mol^{-1}, respectively. The Lennard-Jones potential which was not used during any refinement stage, was -526.2 ± 16.8 kcal mol^{-1} for the final structures. Ramachandran plot analysis of the final structures (residues 727-828) with Procheck-NMR [Laskowski *et al.*, *J. Biolmol. NMR* **8**:477-486 (1996)] showed that 71.0 ± 0.6%, 23.8 ± 0.6%, 3.5 ± 0.2%, and 1.7 ± 0.2% of the non-Gly and non-Pro residues were in the most favorable, additionally allowed, generously allowed, and disallowed regions, respectively. The corresponding values for the residues in the four α-helices (residues 727-743, 770-776, 785-802, and 807-827) were 88.9 ± 0.4%, 11.0 ± 0.4%, 0.1 ± 0.1%, and 0.0 ± 0.0%, respectively. The structure of the bromodomain/acetyl-histamine complex was determined using the free form structure and additional 25 intermolecular and 5 intra-ligand NOE-derived distance restraints.

Site-directed mutagenesis: Mutant proteins were prepared using the QuickChange site-directed mutagenesis kit (Stratagene). The presence of appropriate mutations was confirmed by DNA sequencing.

Ligand titration: Ligand titration experiments were performed by recording a series of 2D ^{15}N- and ^{13}C-HSQC spectra on the uniformly ^{15}N-, and $^{15}N/^{13}C$-labelled bromodomain (~0.3mM), respectively, in the presence of different amounts of ligand concentration ranging from 0 to approximately 2.0 mM. The protein sample and the stock solutions of the ligands were all prepared in the same aqueous buffer containing 100mM phosphate and 5mM perdeuterated DTT at pH 6.5.

The full length nucleic acid sequence of the human p300/CBP-associated factor (P/CAF) was obtained from GenBank. Accession No: U57317.2 (SEQ ID NO:1) :

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   1 ggggccgcgt cgacgcggaa aagaggccgt gggggggcctc ccagcgctgg cagacaccgt
  61 gaggctggca gccgccggca cgcacaccta gtccgcagtc ccgaggaaca tgtccgcagc
 121 cagggcgcgg agcagagtcc cgggcaggag aaccaaggga gggcgtgtgc tgtggcggcg
 181 gcggcagcgg cagcggagcc gctagtcccc tccctcctgg gggagcagct gccgccgctg
 241 ccgccgccgc caccaccatc agcgcgcggg gcccggccag agcgagccgg gcgagcggcg
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301 cgctaggggg agggcggggg cggggagggg ggtgggcgaa gggggcggga gggcgtgggg
361 ggagggtctc gctctcccga ctaccagagc ccgagggaga ccctggcggc ggcggcggcg
421 cctgacactc ggcgcctcct gccgtgctcc ggggcggcat gtccgaggct ggcggggccg
481 ggccgggcgg ctgcggggca ggagccgggg caggggccgg gcccggggcg ctgccccccgc
541 agcctgcggc gcttccgccc gcgcccccgc agggctcccc ctgcgccgct gccgccgggg
601 gctcgggcgc ctgcggtccg gcgacggcag tggctgcagc gggcacggcc gaaggaccgg
661 gaggcggtgg ctcggcccga atcgccgtga agaaagcgca actacgctcc gctccgcggg
721 ccaagaaact ggagaaactc ggagtgtact ccgcctgcaa ggccgaggag tcttgtaaat
781 gtaatggctg gaaaaaccct aacccctcac ccactccccc cagagccgac ctgcagcaaa
841 taattgtcag tctaacagaa tcctgtcgga gttgtagcca tgccctagct gctcatgttt
901 cccacctgga gaatgtgtca gaggaagaaa tgaacagact cctgggaata gtattggatg
961 tggaatatct ctttacctgt gtccacaagg aagaagatgc agataccaaa caagtttatt
1021 tctatctatt taagctcttg agaaagtcta ttttacaaag aggaaaacct gtggttgaag
1081 gctctttgga aaagaaaccc ccatttgaaa aacctagcat tgaacagggt gtgaataact
1141 ttgtgcagta caaatttagt cacctgccag caaaagaaag gcaaacaata gttgagttgg
1201 caaaaatgtt cctaaaccgc atcaactatt ggcatctgga ggcaccatct caacgaagac
1261 tgcgatctcc caatgatgat atttctggat acaaagagaa ctacacaagg tggctgtgtt
1321 actgcaacgt gccacagttc tgcgacagtc tacctcggta cgaaaccaca caggtgtttg
1381 ggagaacatt gcttcgctcg gtcttcactg ttatgaggcg acaactcctg gaacaagcaa
1441 gacaggaaaa agataaactg cctcttgaaa aacgaactct aatcctcact catttcccaa
1501 aatttctgtc catgctagaa gaagaagtat atagtcaaaa ctctcccatc tgggatcagg
1561 attttctctc agcctcttcc agaaccagcc agctaggcat ccaaacagtt atcaatccac
1621 ctcctgtggc tgggacaatt tcatacaatt caacctcatc ttcccttgag cagccaaacg
1681 cagggagcag cagtcctgcc tgcaaagcct cttctggact tgaggcaaac ccaggagaaa
1741 agaggaaaat gactgattct catgttctgg aggaggccaa gaaaccccga gttatggggg
1801 atattccgat ggaattaatc aacgaggtta tgtctaccat cacggaccct gcagcaatgc
1861 ttggaccaga gaccaatttt ctgtcagcac actcggccag ggatgaggcg gcaaggttgg
1921 aagagcgcag gggtgtaatt gaatttcacg tggttggcaa ttccctcaac cagaaaccaa
1981 acaagaagat cctgatgtgg ctggttggcc tacagaacgt tttctcccac cagctgcccc
2041 gaatgccaaa agaatacatc acacggctcg tctttgaccc gaaacacaaa acccttgctt
2101 taattaaaga tggccgtgtt attggtggta tctgtttccg tatgttccca tctcaaggat
2161 tcacagagat tgtcttctgt gctgtaacct caaatgagca agtcaagggc tatggaacac
2221 acctgatgaa tcatttgaaa gaatatcaca taaagcatga catcctgaac ttcctcacat
2281 atgcagatga atatgcaatt ggatacttta agaaacaggg tttctccaaa gaaattaaaa
2341 tacctaaaac caaatatgtt ggctatatca aggattatga aggagccact ttaatgggat
2401 gtgagctaaa tccacggatc ccgtacacag aattttctgt catcattaaa aagcagaagg
2461 agataattaa aaaactgatt gaaagaaaac aggcacaaat tcgaaaagtt taccctggac
2521 tttcatgttt taaagatgga gttcgacaga ttcctataga aagcattcct ggaattagag
2581 agacaggctg gaaaccgagt ggaaaagaga aaagtaaaga gcccagagac cctgaccagc
2641 tttacagcac gctcaagagc atcctccagc aggtgaagag ccatcaaagc gcttggccct
2701 tcatggaacc tgtgaagaga acagaagctc caggatatta tgaagttata aggttcccca
2761 tggatctgaa aaccatgagt gaacgcctca agaataggta ctacgtgtct aagaaattat
2821 tcatggcaga cttacagcga gtctttacca attgcaaaga gtacaacgcc gctgagagtg
2881 aatactacaa atgtgccaat atcctggaga aattcttctt cagtaaaatt aaggaagctg
```

```
2941 gattaattga caagtgattt ttttccccc tctgcttctt agaaactcac caagcagtgt
3001 gcctaaagca aggt
```

The full length protein sequence of the human p300/CBP-associated factor (P/CAF) was obtained from GenBank. Accession No: U57317.2, (SEQ ID NO:2):

```
1   MSEAGGAGPG GCGAGAGAGA GPGALPPQPA ALPPAPPQGS PCAAAAGGSG ACGPATAVAA
61  AGTAEGPGGG GSARIAVKKA QLRSAPRAKK LEKLGVYSAC KAEESCKCNG WKNPNPSPTP
121 PRADLQQIIV SLTESCRSCS HALAAHVSHL ENVSEEEMNR LLGIVLDVEY LFTCVHKEED
181 ADTKQVYFYL FKLLRKSILQ RGKPVVEGSL EKKPPFEKPS IEQGVNNFVQ YKFSHLPAKE
241 RQTIVELAKM FLNRINYWHL EAPSQRRLRS PNDDISGYKE NYTRWLCYCN VPQFCDSLPR
301 YETTQVFGRT LLRSVFTVMR RQLLEQARQE KDKLPLEKRT LILTHFPKFL SMLEEEVYSQ
361 NSPIWDQDFL SASSRTSQLG IQTVINPPPV AGTISYNSTS SSLEQPNAGS SSPACKASSG
421 LEANPGEKRK MTDSHVLEEA KKPRVMGDIP MELINEVMST ITDPAAMLGP ETNFLSAHSA
481 RDEAARLEER RGVIEFHVVG NSLNQKPNKK ILMWLVGLQN VFSHQLPRMP KEYITRLVFD
541 PKHKTLALIK DGRVIGGICF RMFPSQGFTE IVFCAVTSNE QVKGYGTHLM NHLKEYHIKH
601 DILNFLTYAD EYAIGYFKKQ GFSKEIKIPK TKYVGYIKDY EGATLMGCEL NPRIPYTEFS
661 VIIKKQKEII KKLIERKQAQ IRKVYPGLSC FKDGVRQIPI ESIPGIRETG WKPSGKEKSK
721 EPRDPDQLYS TLKSILQQVK SHQSAWPFME PVKRTEAPGY YEVIRFPMDL KTMSERLKNR
781 YYVSKKLFMA DLQRVFTNCK EYNAAESEYY KCANILEKFF FSKIKEAGLI DK
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Results

The P/CAF bromodomain represents an extensive family of bromodomains (Figure 1). A large number of long-range nuclear Overhauser enhancement (NOE)-derived distance restraints were identified in the NMR data of the P/CAF bromodomain, yielding a well-defined three-dimensional structure (Figures 2A -2D). Table 1 shows the NMR chemical shift assignment of the P/CAF bromodomain. Table 2 shows the Unambiguous NOE-derived distance restraints. Table 3 shows the Ambiguous NOE-derived distance restraints. Table 4 shows the Hydrogen bond restraints. The NMR structure coordinates of the P/CAF bromodomain in the free and complexed to acetyl-histamine are shown in Tables 5 and 6, respectively.

The structure consists of a four-helix bundle (helices α_Z, α_A, α_B, and α_C) with a left-handed twist, and a long intervening loop between helices α_Z and α_A (termed the ZA loop, Figure 2E). The four amphipathic α-helices are packed tightly against one another in an antiparallel manner, with crossing angles for adjacent helices of ~16-20°. The up-and-down four-helix bundle can adapt two topological folds with opposite

handedness (Figures 2F-2G). The right-handed four-helix bundle fold occurs more commonly and is seen in proteins such as hemerythrin and cytochrome b_{562}. The left-handed fold of the bromodomain structure is less common, but also observed in proteins such as cytochrome b_5 and T4 lysozyme [Richardson, J., *Adv.Protein Chem.*, **34**:167-339 (1989); Presnell and Cohen, *Proc. Natl. Acad. Sci. USA* **86**:6592-6596 (1989)]. This topological difference arises from the orientation of the loop between the first two helices (Fig. 2F-2G). The right-handed four-helix bundle proteins have a relatively short hairpin-like connection between the first two helices, which makes the "preferred" turn to the right at the top of the first helix [Richardson, J., *Adv.Protein Chem.*, **34**:167-339 (1989); Presnell and Cohen, *Proc. Natl. Acad. Sci. USA* **86**:6592-6596 (1989); Weber and Salemme, *Nature* **287**:82-84 (1980)]. In contrast, proteins with the left-handed fold usually have a long loop after the first helix and often contain additional secondary structural elements at the base of the helix bundle [Richardson, J., *Adv.Protein Chem.*, **34**:167-339 (1989); Presnell and Cohen, *Proc. Natl. Acad. Sci. USA* **86**:6592-6596 (1989)]. In the bromodomain structure, this long ZA loop has a defined conformation and is packed against the loop between helices α_B and α_C (termed the BC loop) to form a hydrophobic pocket. These tertiary interactions between the two loops appear to favor the left turn of the ZA loop, resulting in the left-handed four-helix bundle fold of the bromodomain. The hydrophobic pocket formed by loops ZA and BC is lined by residues Val752, Ala757, Tyr760, Val763, Tyr802 and Tyr809 (Fig. 2H), and appears to be a site for protein-protein interactions (see below). The pocket is located at one end of the four-helix bundle, opposite to the N- and C-termini of the protein. Interestingly, the ZA loop varies in length amongst different bromodomains, but almost always contains residues corresponding to Phe748, Pro751, Pro758, Tyr760, and Pro767 (Figure 1). The conservation of these residues within the ZA loop as well as residues within the α-helical regions implies a similar left-handed four-helix bundle structure for the large family of bromodomains (Fig. 1).

The modular bromodomain structure supports the idea that bromodomain can act as a functional unit for protein-protein interactions. The observation that bromodomains are found in nearly all known nuclear HATs (A-type) that are known to promote transcription-related acetylation of histones on specific lysine residues, but not present in cytoplasmic HATs (B-type), prompted the determination of whether bromodomains

can interact with acetyl-lysine (AcK). The NMR titration of the P/CAF bromodomain were performed with a peptide (SGRGKGG-AcK-GLGK) derived from histone H4, in which Lys8 is acetylated (Lys8 is the major acetylation site in H4 for GCN5, a yeast homologue of P/CAF). Remarkably, the bromodomain could indeed bind the AcK peptide. Moreover, this interaction appeared to be specific, based on the ^{15}N-HSQC spectra which showed that only a limited number of residues underwent chemical shift changes as a function of peptide concentration (Figure 3A). Conversely, the NMR titration of the bromodomain with a non-acetylated, but otherwise identical H4 peptide, showed no noticeable chemical shift changes, demonstrating that the interaction between the bromodomain and the lysine-acetylated H4 peptide was dependent upon acetylation of lysine. The dissociation constant (K_D) for the AcK peptide was estimated to be 346 ± 54 μM. This binding is likely reinforced through additional interactions between bromodomain-containing proteins and target proteins. Notably, many chromatin-associated proteins contain two or multiple bromodomains (Figure 1). Indeed, binding with another lysine-acetylated peptide (RKSTGG-AcK-APRKQ) derived from the major acetylation site on histone H3 (residues 9-20) was also observed. Together, these data demonstrate that the P/CAF bromodomain has the ability to bind AcK peptides in an acetylation dependent manner.

Intriguingly, the bromodomain residues that exhibited the most significant ^{1}H and ^{15}N chemical shift changes on peptide binding are located near the hydrophobic pocket between the ZA and BC loops (Figure 3B). Because a similar pattern of amide chemical shift changes was observed with the two different AcK-containing peptides, it was surmised that the hydrophobic cavity is the primary binding site for AcK. This hypothesis was further supported by titration with acetyl-histamine, which mimics the chemical structure of the AcK side-chain (Figure 3C). Both ^{15}N- and ^{13}C-HSQC spectra showed that interaction with acetyl-histamine was also acetylation-dependent, involving the same set of residues that showed chemical shift perturbations with similar concentration dependence. It should be noted that the bromodomain did not bind to the amino acids acetyl-lysine or acetyl-histidine alone, possibly due to the presence of the charged amino, carboxyl, or caboxylate group adjacent to the acetyl moiety (Figure 3C). Taken together, these results strongly suggest that the P/CAF

bromodomain can interact with acetyl-lysine-containing proteins in a specific manner, and that this interaction is localized to the bromodomain hydrophobic cavity.

To identify the key residues involved in bromodomain-AcK recognition, the NMR structure of the P/CAF bromodomain in complex with acetyl-histamine was elucidated. As anticipated, the acetylated moiety binds in the bromodomain hydrophobic pocket (Figure 4). The intermolecular interactions are largely hydrophobic in nature, with the methyl group of acetyl-histamine making extensive contacts with the side-chains of Val752, Ala757, and Tyr760, and the methylene groups of acetyl-histamine displaying specific NOEs to Val752, Ala757, Tyr760, Tyr802, and Tyr809. No intermolecular NOEs were observed for the imidazole ring of acetyl-histamine. From the spectral analysis it is clear that the structure of the bromodomain is very similar in both the free and complex forms.

It is worth noting that the bromodomain-AcK recognition is reminiscent of the interactions between the histone acetyltransferase Hat1 and acetyl-CoA. Although the binding pockets of these two otherwise structurally unrelated proteins are composed of different secondary structural elements, the nature of acetyl-lysine recognition has striking similarities. In particular, Tyr809, Tyr802, Tyr760, and Val752 in the bromodomain appear to be related to Phe220, Phe261, Val254, and Ile217 of Hat1, respectively, in their interactions with the acetyl moiety. This observation may suggest an evolutionary convergent mechanism of acetyl-lysine recognition between bromodomains and histone acetyltransferases.

To determine the relative contributions of residues within the hydrophobic cavity in bromodomain-AcK binding, site-directed mutagenesis was used to alter residues Tyr809, Tyr802, Tyr760, and Val752 (Table 7).

Table 7. Structural and Functional Analysis of the P/CAF Bromodomain Mutants

Bromodomain Proteins	Structural Integrity [a]	H4 AcK-Peptide Binding K_D (μM) [b]
Wild-Type	++++	346 ± 54
Tyr809Ala	++++	No Binding [c]
Tyr802Ala	+++	> 10,000 [d]
Tyr760Ala	+++	> 10,000
Val752Ala	++	> 10,000

a. The effects of mutations on the structural integrity of the bromodomain were assessed by using the ^{15}N-HSQC spectra. The amide ^{1}H/^{15}N resonances of the mutant proteins were compared to those of the wild-type bromodomain to determine if the particular mutations lead to global or local structure disruption. Severe line-broadening of the amide resonances would indicate protein conformational exchange due to a decrease of structure stability resulting from point mutations. Structural integrity of the mutant proteins is expressed here relative to that of the wild-type, using the signs of "++++" for as stable as the wild-type, "+++" for mildly destabilized, "++" for moderately destabilized, and "–" for completely unfolded.

b. The ligand binding affinity (K_D) of the bromodomain proteins was estimated by following chemical shift changes of amide peaks in the ^{15}N-HSQC spectra as a function of the ligand concentration.

c. No detectable ligand binding observed in the NMR titration.

d. Ligand binding affinity was significantly reduced and beyond the limit for reliable measurements by NMR titration.

Substitution of Ala for Tyr809 completely abrogated the bromodomain binding to the lysine-acetylated H4 peptide, while the Tyr802Ala, Tyr760Ala, and Val752Ala mutants had significantly reduced ligand binding affinity. To assess whether these mutations disrupted the overall bromodomain fold, the ^{15}N-HSQC spectra of the mutants was compared to that of the wild-type protein. For the Tyr809Ala mutant, the amide chemical shifts were only affected for a few residues near the mutation site. However, mutations of the other residues in the hydrophobic binding pocket perturbed the local protein conformation to greater extents, particularly the ZA loop (Table 7). Thus, the NMR structural analysis and the mutagenesis studies show that Tyr809, which is structurally supported by Trp746 and Asn803 (Fiure 4), is essential for the bromodomain interaction with the acetyl group of acetyl-lysine, while residues of Tyr802, Tyr760, and Val752 likely play both structural and functional roles in the recognition. These residues are highly conserved throughout the bromodomain family (Figure 1), suggesting that recognition of acetyl-lysine may be a feature of bromodomains, in general. Therefore, Val752, Ala757, Tyr760, Tyr802, Asn803, and Tyr809 are key amino acid residues for the P/CAF bromodomain binding to acetyl-lysine.

Table 8:Amino Acid Sequences of Bromodomains Identified in Figure 1

PROTEIN **BD**	SEQ ID NO:	GenBank Acc. No.	PROTEIN **BD**	SEQ ID NO:	GenBank Acc. No.
hsp/CAF	7	U57317	dmFSH-2	25	
hsGCN5	8	U57136	scBDF1-2	26	
ttP55	9	U47321	hsBR140	27	JC2069
scGCN5	10	Q03330	hsSMAP	28	X87613
hsP300	11	A54277	ggPB1-1	29	X90849
hsCBP	12	S39162	ggPB1-2	30	
mmCBP	13	S39161	ggPB1-3	31	
ceYNJ1	14	P34545	ggPB1-4	32	
hsCCG1-1	15	P21675	ggPB1-5	33	
msCCG1-1	16	D26114	spBRO-1	34	S54260
hsCCG1-2	17		spBRO-2	35	
msCCG1-2	18		hsSNF2a	36	S45251
hsRing3-1	19	P25440	hsBRG1	37	S39039
hsORFX-1	20	D26362	ggBRM	38	X91638
dmFSH-1	21	P13709	ggBRG1	39	X91637
scBDF1-1	22	P35817	hsTIF1b	40	X97548
hsRing3-2	23		mmTIF1b	41	X99644
hsORFX-2	24		mmTIF1a	42	S78219

The present invention is not to be limited in scope by the specific embodiments described herein. Indeed, various modifications of the invention in addition to those described herein will become apparent to those skilled in the art from the foregoing description and the accompanying figures. Such modifications are intended to fall within the scope of the appended claims.

It is further to be understood that all base sizes or amino acid sizes, and all molecular weight or molecular mass values, given for nucleic acids or polypeptides are approximate, and are provided for description.

Various publications are cited herein, the disclosures of which are hereby incorporated by reference herein in their entireties.

WHAT IS CLAIMED IS:

1. An isolated nucleic acid encoding a peptide consisting of about 21 to 40 amino acids comprising a ZA loop of a bromodomain comprising the amino acid sequence of SEQ ID NO:3.

2. The isolated nucleic acid of Claim 1 further comprising a heterologous nucleotide sequence.

3. An isolated nucleic acid encoding a peptide consisting of about 21 to 40 amino acids comprising a ZA loop of a bromodomain, wherein the bromodomain has an amino acid sequence selected from the group consisting of SEQ ID NOs. 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36 , 37, 38, 39, 40, 41, and 42.

4. The isolated nucleic acid of Claim 3 further comprising a heterologous nucleotide sequence.

5. A peptide consisting of about 21 to 40 amino acids comprising a ZA loop of a bromodomain comprising the amino acid sequence of SEQ ID NO:3.

6. A fusion protein or peptide comprising the peptide of Claim 5.

7. A peptide consisting of about 21 to 40 amino acids comprising a ZA loop of a bromodomain, wherein the bromodomain has an amino acid sequence selected from the group consisting of SEQ ID NOs. 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36 , 37, 38, 39, 40, 41, and 42.

8. A fusion protein or peptide comprising the peptide of Claim 7.

9. An antibody raised against the peptide of Claim 7 or raised against an antigenic fragment thereof.

10. An antibody raised against the peptide of Claim 5.

11. A method of identifying a compound that modulates the affinity of a bromodomain for a ligand that comprises an acetyl-lysine,

said method comprising:

(a) contacting the bromodomain and the ligand in the presence of the compound, wherein the bromodomain and the ligand bind in the absence of the compound; and

(b) measuring the affinity of the bromodomain for the ligand; wherein a compound is identified as a compound that modulates the affinty of the bromodomain for the ligand when there is a change in the affinity of the bromodomain for the ligand in the presence of the compound.

12. The method of Claim 11, wherein the affinity of the bromodomain for the ligand increases in the presence of the compound and wherein the compound is identified as a bromodomain-ligand complex promoting agent.

13. The method of Claim 11, wherein the affinity of the bromodomain for the ligand decreases in the presence of the compound and the compound is identified as an inhibitor.

14. The method of Claim 11, wherein the compound is selected by performing rational drug design with the set of atomic coordinates obtained from one or more of

Tables 1-6, wherein said selecting is performed in conjunction with computer modeling.

15. The method of Claim 11, wherein the compound is selected by performing rational drug design with the set of atomic coordinates obtained from a set of atomic coordinates defining the three-dimensional structure of a bromodomain consisting of the amino acid sequence of SEQ ID NO:7, wherein said selecting is performed in conjunction with computer modeling.

16. A method of identifying a compound that modulates the stability of a bromodomain-acetyl-lysine binding complex comprising:

(a) contacting the bromodomain-acetyl-lysine binding complex in the presence of the compound wherein the bromodomain-acetyl-lysine binding complex forms in the absence of the compound; and

(c) measuring the stability of the bromodomain-acetyl-lysine binding complex; wherein a compound is identified as a compound that modulates the stability of the bromodomain-acetyl-lysine binding complex, when there is a change in the stability of the bromodomain-acetyl-lysine binding complex in the presence of the compound.

17. The method of Claim 16, wherein the stability of the bromodomain-acetyl-lysine binding complex increases in the presence of the compound and wherein the compound is identified as a stabilizing agent.

18. The method of Claim 16, wherein the stability of the bromodomain-acetyl-lysine binding complex decreases in the presence of the compound and the compound is identified as an inhibitor.

19. The method of Claim 16, wherein the compound is selected by performing rational drug design with the set of atomic coordinates obtained from one or more of Tables 1-6, wherein said selecting is performed in conjunction with computer modeling.

20. The method of Claim 16, wherein the compound is selected by performing rational drug design with the set of atomic coordinates obtained from a set of atomic coordinates defining the three-dimensional structure of a bromodomain consisting of the amino acid sequence of SEQ ID NO:7, wherein said selecting is performed in conjunction with computer modeling.

21. A method of identifying a binding partner for a protein that comprises an acetyl-lysine said method comprising:

(a) contacting the protein with a polypeptide comprising a bromodomain; and

(b) determining whether the polypeptide binds to the protein; wherein a binding partner for a protein is identified when polypeptide binds to the protein.

22. The method of Claim 21 wherein the bromodomain has an amino acid sequence from selected from the group consisting of SEQ ID NOs. 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36 , 37, 38, 39, 40, 41 and 42.

23. An agent that can inhibit the binding of a bromodomain with a protein comprising an acetyl-lysine selected from the group consisting of : ISYGR-*AcK*-KRRQRR (SEQ ID NO:4), ARKSTGG-A*cK*-APRKQL (SEQ ID NO:5) and QSTSRHK-*AcK*-LMFKTE (SEQ ID NO:6).

ABSTRACT OF THE INVENTION

The present invention provides the structural determination of a bromodomain determined by NMR spectroscopy. The present invention also provides a binding partner for the bromodomain. In addition, the present invention provides methodology for related drug discovery using high throughput drug screening or structure based rational drug design using the three-dimensional data.

Table 1

NMR Chemical Shift Assignment of the P/CAF Bromodomain

```
RES_ID          715
RES_TYPE        GLY
SPIN_SYSTEM_ID  1
HETEROGENEITY   100
END_RES_DEF

RES_ID          716
RES_TYPE        SER
SPIN_SYSTEM_ID  2
HETEROGENEITY   100
END_RES_DEF

RES_ID          717
RES_TYPE        HIS
SPIN_SYSTEM_ID  3
HETEROGENEITY   100
END_RES_DEF

RES_ID          718
RES_TYPE        MET
SPIN_SYSTEM_ID  4
HETEROGENEITY   100
END_RES_DEF

RES_ID          719
RES_TYPE        SER
SPIN_SYSTEM_ID  5
HETEROGENEITY   100
END_RES_DEF

RES_ID          720
RES_TYPE        LYS
SPIN_SYSTEM_ID  6
HETEROGENEITY   100
  CA  56.296000
  HA  4.361000
  CB  33.140000
  HB1  1.882000
  HB2  1.684000
  CG  25.430000
  HG1  1.585000
  HG2  1.433000
  CD  29.834000
  HD1  1.703000
  CE  41.960000
  HE1  3.003000
END_RES_DEF

RES_ID          721
RES_TYPE        GLU
SPIN_SYSTEM_ID  7
HETEROGENEITY   100
  N  122.990000
  HN  8.317000
  CA  54.620000
  HA  4.540000
  CB  29.830000
  HB1  2.024000
  HB2  1.893000
  CG  35.893000
  HG1  2.271000
END_RES_DEF

RES_ID          722
RES_TYPE        PRO
SPIN_SYSTEM_ID  8
HETEROGENEITY   100
  CA  63.430000
  HA  4.393000
  CB  32.030000
  HB1  2.224000
  HB2  1.880000
  CG  27.630000
  HG1  2.028000
  CD  50.760000
  HD2  3.656000
  HD1  3.800000
END_RES_DEF

RES_ID          723
RES_TYPE        ARG
SPIN_SYSTEM_ID  9
HETEROGENEITY   100
  N  121.192000
  HN  8.416000
  CA  63.430000
  HA  4.331000
  CB  30.930000
  HB1  1.815000
  HB2  1.762000
  CG  27.630000
  HG1  1.681000
  CD  43.603000
  HD1  3.161000
END_RES_DEF

RES_ID          724
RES_TYPE        ASP
SPIN_SYSTEM_ID  10
HETEROGENEITY   100
  N  122.012000
  HN  8.273000
  CA  52.415000
  HA  4.874000
  CB  41.400000
  HB1  2.754000
  HB2  2.692000
END_RES_DEF

RES_ID          725
RES_TYPE        PRO
SPIN_SYSTEM_ID  11
HETEROGENEITY   100
  CA  65.080000
  HA  4.329000
  CB  32.590000
  HB1  2.326000
  HB2  1.973000
  CG  27.632000
  HG1  2.028000
  CD  51.310000
  HD1  3.866000
END_RES_DEF

RES_ID          726
RES_TYPE        ASP
SPIN_SYSTEM_ID  12
HETEROGENEITY   100
  N  119.716000
  HN  8.397000
  CA  55.720000
  HA  4.692000
  CB  40.550000
  HB1  2.792000
  HB2  2.730000
END_RES_DEF

RES_ID          727
RES_TYPE        GLN
SPIN_SYSTEM_ID  13
HETEROGENEITY   100
  N  121.356000
  HN  8.196000
  CA  55.920000
  HA  4.163000
  CB  28.730000
  HB1  2.148000
  CG  34.240000
  HG1  2.524000
  HG2  2.371000
END_RES_DEF

RES_ID          728
RES_TYPE        LEU
SPIN_SYSTEM_ID  14
HETEROGENEITY   100
  N  121.356000
  HN  8.210000
  CA  58.473000
  HA  4.045000
  CB  41.400000
  HB1  1.847000
  HB2  1.555000
  CG  27.080000
  HG  1.480000
  CD1  25.970000
  HD1#  0.794000
  CD2  23.226000
  HD2#  0.786000
END_RES_DEF

RES_ID          729
RES_TYPE        TYR
SPIN_SYSTEM_ID  15
HETEROGENEITY   100
  N  119.060000
  HN  8.021000
  CA  62.320000
  HA  4.038000
  CB  38.640000
  HB1  3.211000
  HB2  3.024000
  CD1  134.350000
  HD1  7.053000
  CE1  119.481000
  HE1  6.882000
END_RES_DEF

RES_ID          730
RES_TYPE        SER
SPIN_SYSTEM_ID  16
HETEROGENEITY   100
  N  112.173000
  HN  8.167000
  HA  3.920000
  HB1  3.995000
END_RES_DEF

RES_ID          731
RES_TYPE        THR
SPIN_SYSTEM_ID  17
HETEROGENEITY   100
  N  120.372000
  HN  8.059000
  CA  66.730000
  HA  3.924000
  CB  68.930000
  HB  4.247000
  CG2  21.570000
  HG2#  1.142000
END_RES_DEF

RES_ID          732
RES_TYPE        LEU
SPIN_SYSTEM_ID  18
HETEROGENEITY   100
  N  120.536000
  HN  8.460000
  CA  57.920000
  HA  3.289000
  CB  39.750000
  HB1  1.532000
  HB2  0.294000
  CG  24.880000
  HG  1.683000
  CD1  25.429000
  HD1#  0.469000
  CD2  19.921000
  HD2#  -0.193000
END_RES_DEF

RES_ID          733
RES_TYPE        LYS
SPIN_SYSTEM_ID  19
HETEROGENEITY   100
  N  118.568000
  HN  8.563000
  CA  60.125000
  HA  3.679000
  CB  32.588000
  HB1  1.729000
  HB2  1.360000
  CG  24.880000
  HG1  1.280000
  CD  29.835000
  HD1  1.585000
  CE  41.960000
  HE1  2.918000
END_RES_DEF

RES_ID          734
RES_TYPE        SER
SPIN_SYSTEM_ID  20
HETEROGENEITY   100
  N  113.157000
  HN  7.540000
  CA  61.227000
  HA  4.281000
  CB  63.879000
  HB1  4.060000
END_RES_DEF

RES_ID          735
RES_TYPE        ILE
SPIN_SYSTEM_ID  21
HETEROGENEITY   100
  N  120.700000
  HN  7.951000
  CA  65.080000
  HA  3.786000
  CB  38.095000
  HB  1.879000
  CG1  28.733000
  HG11  1.748000
  HG12  1.052000
  CG2  17.168000
  HG2#  1.003000
  CD1  13.863000
  HD1#  0.619000
END_RES_DEF

RES_ID          736
RES_TYPE        LEU
SPIN_SYSTEM_ID  22
HETEROGENEITY   100
  N  119.880000
  HN  8.841000
  CA  58.473000
  HA  4.090000
  CB  41.950000
  HB1  2.090000
  HB2  1.703000
  CG  27.330000
  HG  1.759000
  CD1  26.530000
  HD1#  1.061000
  CD2  23.776000
  HD2#  0.977000
END_RES_DEF

RES_ID          737
RES_TYPE        GLN
SPIN_SYSTEM_ID  23
HETEROGENEITY   100
  N  117.256000
  HN  8.505000
  CA  59.020000
  HA  4.032000
  CB  28.182000
  HB1  2.327000
  HB2  2.263000
  CG  34.240000
  HG1  2.536000
  HG2  2.461000
END_RES_DEF

RES_ID          738
RES_TYPE        GLN
SPIN_SYSTEM_ID  24
HETEROGENEITY   100
  N  118.896000
  HN  8.033000
  CA  59.574000
  HA  4.196000
  CB  29.835000
  HB1  2.482000
  HB2  2.469000
  CG  35.342000
  HG1  2.840000
  HG2  2.467000
  NE2  110.369000
  HE21  7.022000
  HE22  6.916000
END_RES_DEF

RES_ID          739
RES_TYPE        VAL
SPIN_SYSTEM_ID  25
HETEROGENEITY   100
  N  119.716000
  HN  8.526000
  CA  67.830000
  HA  3.844000
  CB  32.030000
  HB  2.384000
  CG1  23.330000
  HG1#  1.183000
  CG2  22.120000
  HG2#  1.033000
END_RES_DEF

RES_ID          740
RES_TYPE        LYS
SPIN_SYSTEM_ID  26
HETEROGENEITY   100
  N  114.633000
  HN  8.572000
  CA  59.574000
  HA  3.886000
  CB  32.380000
  HB1  1.873000
  HG1  1.022000
  HD1  1.520000
END_RES_DEF

RES_ID          741
RES_TYPE        SER
```

SPIN_SYSTEM_ID 27
HETEROGENEITY 100
N 110.369000
HN 7.557000
CA 59.024000
HA 4.448000
CB 63.980000
HB1 4.004000
END_RES_DEF

RES_ID 742
RES_TYPE HIS
SPIN_SYSTEM_ID 28
HETEROGENEITY 100
N 125.619000
HN 7.536000
CA 58.473000
HA 3.967000
CB 32.588000
HB1 2.990000
HB2 2.799000
CD2 118.930000
HD2 4.978000
CE1 138.755000
HE1 7.522000
END_RES_DEF

RES_ID 743
RES_TYPE GLN
SPIN_SYSTEM_ID 29
HETEROGENEITY 100
N 128.571000
HN 8.543000
CA 59.125000
HA 4.209000
CB 29.834000
HB1 2.111000
CG 33.690000
HG1 2.390000
NE2 112.173000
HE21 7.581000
HE22 6.870000
END_RES_DEF

RES_ID 744
RES_TYPE SER
SPIN_SYSTEM_ID 30
HETEROGENEITY 100
N 119.060000
HN 11.668000
CA 60.125000
HA 4.838000
CB 63.980000
HB1 4.334000
HB2 3.926000
END_RES_DEF

RES_ID 745
RES_TYPE ALA
SPIN_SYSTEM_ID 31
HETEROGENEITY 100
N 117.584000
HN 7.868000
CA 53.510000
HA 4.396000
CB 20.470000
HB# 1.688000
END_RES_DEF

RES_ID 746
RES_TYPE TRP
SPIN_SYSTEM_ID 32
HETEROGENEITY 100
N 116.600000
HN 7.135000
CA 60.691000
HA 4.368000
CB 27.630000
HB1 3.594000
HB2 3.351000
CD1 128.843000
HD1 7.897000
NE1 110.861000
HE1 10.474000
CE3 122.234000
HE3 7.336000
CZ2 116.177000
HZ2 7.382000
CZ3 123.336000
HZ3 7.197000
CH2 126.089000
HH2 7.150000
END_RES_DEF

RES_ID 747
RES_TYPE PRO
SPIN_SYSTEM_ID 33
HETEROGENEITY 100
CA 64.531000
HA 3.756000
CB 29.835000
HB1 0.487000
HB2 -0.783000
CG 26.530000
HG1 0.233000
HG2 -0.931000
CD 50.212000
HD2 1.567000
HD1 2.177000
END_RES_DEF

RES_ID 748
RES_TYPE PHE
SPIN_SYSTEM_ID 34
HETEROGENEITY 100
N 113.321000
HN 7.585000
CA 55.719000
HA 4.930000
CB 39.202000
HB1 3.491000
HB2 2.532000
CD1 133.248000
HD1 7.099000
HE1 7.174000
HZ 7.296000
END_RES_DEF

RES_ID 749
RES_TYPE MET
SPIN_SYSTEM_ID 35
HETEROGENEITY 100
N 117.748000
HN 7.115000
CA 56.820000
HA 4.286000
CB 32.590000
HB1 2.233000
HB2 2.174000
CG 33.140000
HG1 2.851000
CE 17.168000
HE# 2.175000
END_RES_DEF

RES_ID 750
RES_TYPE GLU
SPIN_SYSTEM_ID 36
HETEROGENEITY 100
N 113.813000
HN 7.709000
CA 53.516000
HA 4.849000
CB 31.487000
HB1 2.091000
HB2 1.730000
CG 35.893000
HG1 2.164000
END_RES_DEF

RES_ID 751
RES_TYPE PRO
SPIN_SYSTEM_ID 37
HETEROGENEITY 100
CA 62.879000
HA 4.242000
CB 32.040000
HB1 2.328000
HB2 1.683000
CG 27.080000
HG1 2.126000
HG2 1.978000
CD 50.763000
HD1 3.670000
END_RES_DEF

RES_ID 752
RES_TYPE VAL
SPIN_SYSTEM_ID 38
HETEROGENEITY 100
N 124.450000
HN 8.124000
CA 63.430000
HA 3.553000
CB 32.580000
HB 1.145000
CG1 21.573000
HG1# 0.464000
CG2 21.573000
HG2# 0.169000
END_RES_DEF

RES_ID 753
RES_TYPE LYS
SPIN_SYSTEM_ID 39
HETEROGENEITY 100
N 129.883000
HN 9.045000
CA 56.310000
HA 4.370000
CB 32.880000
HB1 1.873000
HG1 1.435000
HD1 1.673000
HE1 2.985000
END_RES_DEF

RES_ID 754
RES_TYPE ARG
SPIN_SYSTEM_ID 40
HETEROGENEITY 100
N 120.208000
HN 8.054000
END_RES_DEF

RES_ID 755
RES_TYPE THR
SPIN_SYSTEM_ID 41
HETEROGENEITY 100
CA 63.430000
HA 4.038000
CB 68.380000
HB 4.293000
CG2 22.670000
HG2# 1.267000
END_RES_DEF

RES_ID 756
RES_TYPE GLU
SPIN_SYSTEM_ID 42
HETEROGENEITY 100
N 118.732000
HN 7.209000
CA 56.270000
HA 4.448000
CB 30.930000
HB1 2.174000
HB2 2.000000
CG 36.440000
HG1 2.292000
END_RES_DEF

RES_ID 757
RES_TYPE ALA
SPIN_SYSTEM_ID 43
HETEROGENEITY 100
N 122.504000
HN 7.379000
CA 50.220000
HA 4.937000
CB 19.370000
HB# 1.082000
END_RES_DEF

RES_ID 758
RES_TYPE PRO
SPIN_SYSTEM_ID 44
HETEROGENEITY 100
CA 65.080000
HA 4.496000
CB 31.487000
HB1 2.374000
HB2 2.027000
CG 27.632000
HG1 2.122000
HG2 2.038000
CD 50.212000
HD2 3.515000
HD1 3.717000
END_RES_DEF

RES_ID 759
RES_TYPE GLY
SPIN_SYSTEM_ID 45
HETEROGENEITY 100
END_RES_DEF

RES_ID 760
RES_TYPE TYR
SPIN_SYSTEM_ID 46
HETEROGENEITY 100
N 122.504000
HN 7.945000
CA 62.328000
HA 3.536000
CB 39.750000
HB1 2.689000
HB2 2.487000
CD1 133.799000
HD1 5.120000
CE1 118.379000
HE1 6.070000
END_RES_DEF

RES_ID 761
RES_TYPE TYR
SPIN_SYSTEM_ID 47
HETEROGENEITY 100
N 113.157000
HN 8.225000
CA 60.676000
HA 4.101000
CB 37.550000
HB1 3.189000
HB2 2.801000
CD1 134.901000
HD1 7.342000
CE1 118.930000
HE1 6.646000
END_RES_DEF

RES_ID 762
RES_TYPE GLU
SPIN_SYSTEM_ID 48
HETEROGENEITY 100
N 117.912000
HN 7.702000
CA 57.922000
HA 4.209000
CB 29.480000
HB1 2.086000
CG 37.545000
HG1 2.325000
HG2 2.265000
END_RES_DEF

RES_ID 763
RES_TYPE VAL
SPIN_SYSTEM_ID 49
HETEROGENEITY 100
N 115.453000
HN 7.135000
CA 63.430000
HA 4.077000
CB 33.690000
HB 2.015000
CG1 21.020000
HG1# 1.045000
CG2 21.574000
HG2# 0.991000
END_RES_DEF

RES_ID 764
RES_TYPE ILE
SPIN_SYSTEM_ID 50
HETEROGENEITY 100
N 122.832000
HN 7.947000
CA 57.920000
HA 3.916000
CB 34.240000
HB 1.205000
CG1 24.878000
HG11 0.798000
HG12 0.216000
CG2 16.617000
HG2# 0.380000
CD1 9.457000
HD1# 0.537000
END_RES_DEF

RES_ID 765
RES_TYPE ARG
SPIN_SYSTEM_ID 51
HETEROGENEITY 100
N 125.291000
HN 7.749000
CA 57.371000
HA 3.875000
CB 30.936000
HB1 1.388000
HB2 1.211000
CG 27.080000
HG1 1.319000
HG2 1.173000
CD 43.052000
HD1 2.971000
END_RES_DEF

RES_ID 766

```
RES_TYPE         SER
SPIN_SYSTEM_ID   52
HETEROGENEITY    100
  N  116.600000
  HN   8.387000
  CA  54.618000
  HA   4.984000
  CB  38.640000
  HB1  3.034000
  HB2  2.907000
END_RES_DEF

RES_ID           767
RES_TYPE         PRO
SPIN_SYSTEM_ID   53
HETEROGENEITY    100
  CA  63.429000
  HA   4.083000
  CB  32.588000
  HB1  2.209000
  CG  28.180000
  HG1  2.177000
  HG2  1.883000
  CD  50.763000
  HD2  3.390000
  HD1  3.623000
END_RES_DEF

RES_ID           768
RES_TYPE         MET
SPIN_SYSTEM_ID   54
HETEROGENEITY    100
  N  119.060000
  HN   8.430000
  CA  54.067000
  HA   4.935000
  CB  31.487000
  HB1  1.989000
  HB2  1.353000
  CG  30.930000
  HG1  2.690000
  CE  14.414000
  HE#  1.929000
END_RES_DEF

RES_ID           769
RES_TYPE         ASP
SPIN_SYSTEM_ID   55
HETEROGENEITY    100
  N  119.060000
  HN   7.365000
  CA  53.516000
  HA   4.745000
  CB  44.154000
  HB1  2.371000
END_RES_DEF

RES_ID           770
RES_TYPE         LEU
SPIN_SYSTEM_ID   56
HETEROGENEITY    100
  N  116.272000
  HN   9.055000
  CA  57.922000
  HA   4.036000
  CB  41.400000
  HB1  2.095000
  HB2  1.395000
  CG  27.080000
  HG   1.713000
  CD1 27.080000
  HD1# 0.940000
  CD2 22.675000
  HD2# 0.628000
END_RES_DEF

RES_ID           771
RES_TYPE         LYS
SPIN_SYSTEM_ID   57
HETEROGENEITY    100
  N  128.079000
  HN   8.738000
  CA  60.676000
  HA   4.198000
  CB  32.037000
  HB1  2.330000
  HB2  2.224000
  CG  25.280000
  HG1  1.483000
  HG2  1.403000
  CD  30.385000
  HD1  1.793000
  HD2  1.696000
  CE  41.950000
  HE1  2.965000
END_RES_DEF

RES_ID           772
RES_TYPE         THR
SPIN_SYSTEM_ID   58
HETEROGENEITY    100
  N  122.176000
  HN   9.445000
  CA  67.040000
  HA   3.845000
  CB  67.835000
  HB   4.090000
  CG2 22.124000
  HG2# 1.058000
END_RES_DEF

RES_ID           773
RES_TYPE         MET
SPIN_SYSTEM_ID   59
HETEROGENEITY    100
  N  117.912000
  HN   7.882000
  CA  60.676000
  HA   4.319000
  CB  33.342000
  HB1  2.093000
  HB2  1.915000
  CG  33.139000
  HG1  2.621000
  HG2  2.496000
  CE  16.620000
  HE#  1.241000
END_RES_DEF

RES_ID           774
RES_TYPE         SER
SPIN_SYSTEM_ID   60
HETEROGENEITY    100
  N  116.108000
  HN   7.958000
  CA  62.879000
  HA   4.200000
  CB  62.879000
  HB1  4.368000
  HB2  4.040000
END_RES_DEF

RES_ID           775
RES_TYPE         GLU
SPIN_SYSTEM_ID   61
HETEROGENEITY    100
  N  124.471000
  HN   8.150000
  CA  59.570000
  HA   4.045000
  CB  29.280000
  HB1  2.246000
  HB2  2.063000
  CG  36.443000
  HG1  2.345000
  HG2  2.176000
END_RES_DEF

RES_ID           776
RES_TYPE         ARG
SPIN_SYSTEM_ID   62
HETEROGENEITY    100
  N  120.372000
  HN   8.391000
  CA  60.676000
  HA   3.869000
  CB  30.385000
  HB1  2.047000
  HB2  1.076000
  CG  29.284000
  HG1  1.722000
  HG2  0.877000
  CD  44.154000
  HD1  2.578000
  HD2  2.051000
END_RES_DEF

RES_ID           777
RES_TYPE         LEU
SPIN_SYSTEM_ID   63
HETEROGENEITY    100
  N  120.208000
  HN   8.856000
  CA  58.470000
  HA   4.691000
  CB  42.621000
  HB1  2.295000
  HB2  1.925000
  CG  27.080000
  HG   1.832000
  CD1 25.429000
  HD1# 1.067000
  CD2 27.081000
  HD2# 0.871000
END_RES_DEF

RES_ID           778
RES_TYPE         LYS
SPIN_SYSTEM_ID   64
HETEROGENEITY    100
  N  120.372000
  HN   7.958000
  CA  59.574000
  HA   4.333000
  CB  32.588000
  HB1  2.055000
  CG  24.878000
  HG1  1.596000
  CD  29.835000
  HD1  1.804000
  CE  41.951000
  HE1  2.990000
END_RES_DEF

RES_ID           779
RES_TYPE         ASN
SPIN_SYSTEM_ID   65
HETEROGENEITY    100
  N  116.108000
  HN   7.947000
  CA  53.510000
  HA   4.771000
  CB  38.095000
  HB1  3.019000
  HB2  2.773000
  ND2 112.665000
  HD21  7.598000
  HD22  6.969000
END_RES_DEF

RES_ID           780
RES_TYPE         ARG
SPIN_SYSTEM_ID   66
HETEROGENEITY    100
  N  114.141000
  HN   8.158000
  CA  56.821000
  HA   4.405000
  CB  25.429000
  HB1  2.097000
  HB2  2.022000
  CG  27.632000
  HG1  1.539000
  HG2  1.534000
  CD  43.050000
  HD1  3.060000
  HD2  3.024000
END_RES_DEF

RES_ID           781
RES_TYPE         TYR
SPIN_SYSTEM_ID   67
HETEROGENEITY    100
  N  116.764000
  HN   8.222000
  CA  60.125000
  HA   4.064000
  CB  40.850000
  HB1  2.948000
  HB2  2.055000
  CD1 134.350000
  HD1  6.285000
  CE1 118.930000
  HE1  6.709000
END_RES_DEF

RES_ID           782
RES_TYPE         TYR
SPIN_SYSTEM_ID   68
HETEROGENEITY    100
  N  114.633000
  HN   8.014000
  CA  57.920000
  HA   4.528000
  CB  36.443000
  HB1  3.062000
  HB2  2.907000
  CD1 133.248000
  HD1  7.175000
  CE1 120.582000
  HE1  7.286000
END_RES_DEF

RES_ID           783
RES_TYPE         VAL
SPIN_SYSTEM_ID   69
HETEROGENEITY    100
  N  115.780000
  HN   7.698000
  CA  62.330000
  HA   4.083000
  CB  31.500000
  HB   2.321000
  CG1 21.570000
  HG1#  0.944000
  CG2 18.820000
  HG2#  0.823000
END_RES_DEF

RES_ID           784
RES_TYPE         SER
SPIN_SYSTEM_ID   70
HETEROGENEITY    100
  N  111.353000
  HN   7.415000
  CA  55.719000
  HA   4.741000
  CB  66.183000
  HB1  4.200000
  HB2  3.750000
END_RES_DEF

RES_ID           785
RES_TYPE         LYS
SPIN_SYSTEM_ID   71
HETEROGENEITY    100
  CA  59.030000
  HA   4.021000
  CB  31.590000
END_RES_DEF

RES_ID           786
RES_TYPE         LYS
SPIN_SYSTEM_ID   72
HETEROGENEITY    100
  N  120.208000
  HN   8.244000
  CA  59.720000
  HA   4.062000
  CB  30.385000
  HB1  1.779000
  CG  24.530000
  CD  28.182000
  HD1  1.680000
  CE  41.670000
  HE1  3.137000
  HE2  3.045000
END_RES_DEF

RES_ID           787
RES_TYPE         LEU
SPIN_SYSTEM_ID   73
HETEROGENEITY    100
  N  118.732000
  HN   7.422000
  CA  57.922000
  HA   4.213000
  CB  43.603000
  HB1  1.996000
  HB2  1.891000
  CG  27.632000
  HG   1.794000
  CD1 25.979000
  HD1#  0.924000
  CD2 23.776000
  HD2#  0.895000
END_RES_DEF

RES_ID           788
RES_TYPE         PHE
SPIN_SYSTEM_ID   74
HETEROGENEITY    100
  N  118.732000
  HN   6.928000
  CA  60.676000
  HA   3.763000
  CB  39.750000
  HB1  2.945000
  HB2  2.381000
  CD1 133.799000
  HD1  6.400000
  CE1 131.596000
  HE1  6.928000
END_RES_DEF

RES_ID           789
RES_TYPE         MET
SPIN_SYSTEM_ID   75
HETEROGENEITY    100
  N  116.272000
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    HN  8.489000
    CA  59.020000
    HA  3.911000
    CB  32 590000
    HB1  2.318000
    HB2  2.208000
    CG  33.140000
    HG1  2.942000
    HG2  2.611000
    CE  17.168000
    HE#  2.027000
  END_RES_DEF

  RES_ID          790
  RES_TYPE        ALA
  SPIN_SYSTEM_ID  76
  HETEROGENEITY   100
    N  119.716000
    HN  8.000000
    CA  55.170000
    HA  4.084000
    CB  18.270000
    HB#  1.485000
  END_RES_DEF

  RES_ID          791
  RES_TYPE        ASP
  SPIN_SYSTEM_ID  77
  HETEROGENEITY   100
    N  119.716000
    HN  7.376000
    CA  57.371000
    HA  4.371000
    CB  38.646000
    HB1  2.730000
  END_RES_DEF

  RES_ID          792
  RES_TYPE        LEU
  SPIN_SYSTEM_ID  78
  HETEROGENEITY   100
    N  119.550000
    HN  7.363000
    CA  57.922000
    HA  3.398000
    CB  40.299000
    HB1  0.757000
    HB2  0.442000
    CG  27.632000
    HG  0.707000
    CD1  24.327000
    HD1#  0.184000
    CD2  25.979000
    HD2#  0.061000
  END_RES_DEF

  RES_ID          793
  RES_TYPE        GLN
  SPIN_SYSTEM_ID  79
  HETEROGENEITY   100
    N  114.141000
    HN  8.069000
    CA  59.024000
    HA  3.804000
    CB  28.733000
    HB1  2.157000
    HB2  2.097000
    CG  35.342000
    HG1  2.460000
    NE2  111.353000
    HE21  7.319000
    HE22  7.222000
  END_RES_DEF

  RES_ID          794
  RES_TYPE        ARG
  SPIN_SYSTEM_ID  80
  HETEROGENEITY   100
    N  118.568000
    HN  7.382000
    CA  58.473000
    HA  4.078000
    CB  29.835000
    HB1  1.973000
    HB2  1.886000
    CG  27.080000
    HG1  1.742000
    CD  43.603000
    HD1  3.390000
    HD2  3.325000
  END_RES_DEF

  RES_ID          795
  RES_TYPE        VAL
  SPIN_SYSTEM_ID  81
  HETEROGENEITY   100
    N  117.912000
    HN  7.013000
    CA  66.730000
    HA  3.039000
    CB  30.930000
    HB  1.435000
    CG1  22.124000
    HG1#  0.479000
    CG2  21.573000
    HG2#  0.142000
  END_RES_DEF

  RES_ID          796
  RES_TYPE        PHE
  SPIN_SYSTEM_ID  82
  HETEROGENEITY   100
    N  116.928000
    HN  6.357000
    CA  58.470000
    HA  4.161000
    CB  38.096000
    HB1  3.090000
    HB2  2.944000
    CD1  132.147000
    HD1  6.641000
    CE1  131.596000
    HE1  6.456000
    CZ  129.393000
    HZ  6.406000
  END_RES_DEF

  RES_ID          797
  RES_TYPE        THR
  SPIN_SYSTEM_ID  83
  HETEROGENEITY   100
    N  115.289000
    HN  9.047000
    CA  66.734000
    HA  3.838000
    CB  68.380000
    HB  4.210000
    CG2  22.120000
    HG2#  1.296000
  END_RES_DEF

  RES_ID          798
  RES_TYPE        ASN
  SPIN_SYSTEM_ID  84
  HETEROGENEITY   100
    N  120.700000
    HN  8.846000
    CA  55.170000
    HA  4.315000
    CB  38.090000
    HB1  2.985000
    HB2  2.661000
  END_RES_DEF

  RES_ID          799
  RES_TYPE        CYS
  SPIN_SYSTEM_ID  85
  HETEROGENEITY   100
    N  116.928000
    HN  6.893000
    CA  62.157000
    HA  4.405000
    CB  26.530000
    HB1  3.304000
    HB2  3.032000
  END_RES_DEF

  RES_ID          800
  RES_TYPE        LYS
  SPIN_SYSTEM_ID  86
  HETEROGENEITY   100
    N  116.764000
    HN  7.799000
    CA  58.473000
    HA  4.204000
    CB  32.588000
    HB1  1.743000
    CG  25.429000
    HG1  1.313000
    HG2  0.138000
    CD  29.835000
    HD1  1.291000
    CE  41.400000
    HE1  2.486000
    HE2  2.421000
  END_RES_DEF

  RES_ID          801
  RES_TYPE        GLU
  SPIN_SYSTEM_ID  87
  HETEROGENEITY   100
    N  117.912000
    HN  7.945000
    CA  57.992000
    HA  4.250000
    CB  30.385000
    HB1  2.172000
    HB2  2.003000
    CG  36.994000
    HG1  2.407000
    HG2  2.203000
  END_RES_DEF

  RES_ID          802
  RES_TYPE        TYR
  SPIN_SYSTEM_ID  88
  HETEROGENEITY   100
    N  116.600000
    HN  7.744000
    CA  60.676000
    HA  4.369000
    CB  41.400000
    HB1  2.929000
    CD1  134.901000
    HD1  6.989000
    CE1  119.481000
    HE1  6.823000
  END_RES_DEF

  RES_ID          803
  RES_TYPE        ASN
  SPIN_SYSTEM_ID  89
  HETEROGENEITY   100
    N  115.944000
    HN  8.241000
    CA  51.864000
    HA  5.024000
    CB  40.849000
    HB1  3.069000
    HB2  2.907000
    ND2  118.732000
    HD21  8.316000
    HD22  7.809000
  END_RES_DEF

  RES_ID          804
  RES_TYPE        ALA
  SPIN_SYSTEM_ID  90
  HETEROGENEITY   100
  END_RES_DEF

  RES_ID          805
  RES_TYPE        PRO
  SPIN_SYSTEM_ID  91
  HETEROGENEITY   100
    CA  63.980000
    HA  2.422000
    HB1  1.949000
    HG1  1.648000
    HG2  1.558000
    CD  50.762000
    HD2  3.601000
    HD1  3.706000
  END_RES_DEF

  RES_ID          806
  RES_TYPE        GLU
  SPIN_SYSTEM_ID  92
  HETEROGENEITY   100
    N  112.993000
    HN  8.246000
    CA  56.820000
    HA  4.185000
    CB  28.733000
    HB1  2.095000
    HB2  1.973000
    CG  36.270000
    HG1  2.200000
  END_RES_DEF

  RES_ID          807
  RES_TYPE        SER
  SPIN_SYSTEM_ID  93
  HETEROGENEITY   100
    N  115.780000
    HN  8.112000
    CA  58.473000
    HA  4.406000
    CB  66.183000
    HB1  4.393000
    HB2  4.157000
  END_RES_DEF

  RES_ID          808
  RES_TYPE        GLU
  SPIN_SYSTEM_ID  94
  HETEROGENEITY   100
    N  123.488000
    HN  9.061000
    CA  59.574000
    HA  4.232000
    CB  29.835000
    HB1  2.169000
    CG  36.443000
    HG1  2.528000
  END_RES_DEF

  RES_ID          809
  RES_TYPE        TYR
  SPIN_SYSTEM_ID  95
  HETEROGENEITY   100
    N  116.436000
    HN  8.072000
    CA  60.120000
    HA  3.834000
    CB  37.550000
    HB1  3.018000
    HB2  2.738000
    CD1  132.698000
    HD1  6.891000
    CE1  120.032000
    HE1  7.011000
  END_RES_DEF

  RES_ID          810
  RES_TYPE        TYR
  SPIN_SYSTEM_ID  96
  HETEROGENEITY   100
    N  119.880000
    HN  7.356000
    CA  61.777000
    HA  3.819000
    CB  40.300000
    HB1  3.390000
    HB2  2.500000
    CD1  136.553000
    HD1  7.094000
    CE1  119.481000
    HE1  7.000000
  END_RES_DEF

  RES_ID          811
  RES_TYPE        LYS
  SPIN_SYSTEM_ID  97
  HETEROGENEITY   100
    N  118.076000
    HN  8.072000
    CA  60.676000
    HA  4.204000
    CB  32.588000
    HB1  2.091000
    CG  25.979000
    HG1  1.819000
    HG2  1.582000
    CD  29.834000
    HD1  1.813000
    CE  41.963000
    HE1  2.962000
  END_RES_DEF

  RES_ID          812
  RES_TYPE        CYS
  SPIN_SYSTEM_ID  98
  HETEROGENEITY   100
    N  116.764000
    HN  8.520000
    CA  65.087000
    HA  4.202000
    CB  27.080000
    HB1  3.396000
    HB2  3.056000
  END_RES_DEF

  RES_ID          813
  RES_TYPE        ALA
  SPIN_SYSTEM_ID  99
  HETEROGENEITY   100
    N  120.700000
    HN  8.315000
    CA  55.563000
    HA  3.834000
    CB  18.270000
    HB#  1.597000
  END_RES_DEF

  RES_ID          814
  RES_TYPE        ASN
  SPIN_SYSTEM_ID  100
  HETEROGENEITY   100
    N  115.453000
```

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    HN  8.068000
    CA  56.270000
    HA  4.329000
    CB  38.646000
    HB1  2.877000
    HB2  2.834000
  END_RES_DEF

  RES_ID          815
  RES_TYPE        ILE
  SPIN_SYSTEM_ID  101
  HETEROGENEITY   100
    N  119.880000
    HN  7.912000
    CA  65.080000
    HA  3.646000
    CB  39.197000
    HB  1.924000
    CG1  29.284000
    HG11  1.882000
    HG12  1.201000
    CG2  17.718000
    HG2#  1.017000
    CD1  13.863000
    HD1#  0.940000
  END_RES_DEF

  RES_ID          816
  RES_TYPE        LEU
  SPIN_SYSTEM_ID  102
  HETEROGENEITY   100
    N  122.504000
    HN  8.556000
    CA  56.820000
    HA  3.670000
    CB  41.951000
    HB1  1.405000
    HB2  1.199000
    CG  26.530000
    HG  1.580000
    CD1  24.327000
    HD1#  0.701000
    CD2  25.429000
    HD2#  0.696000
  END_RES_DEF

  RES_ID          817
  RES_TYPE        GLU
  SPIN_SYSTEM_ID  103
  HETEROGENEITY   100
    N  120.700000
    HN  8.073000
    CA  60.125000
    HA  3.185000
    CB  29.835000
    HB1  1.720000
    HB2  1.310000
    CG  37.545000
    HG1  2.001000
    HG2  1.922000
  END_RES_DEF

  RES_ID          818
  RES_TYPE        LYS
  SPIN_SYSTEM_ID  104
  HETEROGENEITY   100
    N  117.584000
    HN  7.145000
    CA  59.688000
    HA  4.075000
    CB  32.588000
    HB1  1.929000
    CG  25.644000
    HG1  1.492000
    CD  29.284000
    HD1  1.681000
    CE  41.963000
    HE1  2.964000
  END_RES_DEF

  RES_ID          819
  RES_TYPE        PHE
  SPIN_SYSTEM_ID  105
  HETEROGENEITY   100
    N  121.028000
    HN  7.869000
    CA  61.230000
    HA  4.328000
    CB  39.200000
    HB1  3.133000
    HB2  3.047000
    CD1  133.800000
    HD1  7.180000
  END_RES_DEF

  RES_ID          820
  RES_TYPE        PHE
  SPIN_SYSTEM_ID  106
  HETEROGENEITY   100
    N  120.700000
    HN  9.126000
    CA  60.691000
    HA  3.961000
    CB  38.640000
    HB1  3.289000
    HB2  3.067000
    CD1  133.248000
    HD1  6.904000
    CE1  132.698000
    HE1  7.011000
  END_RES_DEF

  RES_ID          821
  RES_TYPE        PHE
  SPIN_SYSTEM_ID  107
  HETEROGENEITY   100
    N  118.076000
    HN  8.359000
    CA  61.770000
    HA  3.840000
    CB  38.090000
    HB1  3.064000
    CD1  133.248000
    HD1  7.175000
    CE1  132.698000
    HE1  7.294000
    CZ  131.596000
    HZ  7.430000
  END_RES_DEF

  RES_ID          822
  RES_TYPE        SER
  SPIN_SYSTEM_ID  108
  HETEROGENEITY   100
    N  114.961000
    HN  7.906000
    CA  61.773000
    HA  4.200000
    CB  62.879000
    HB1  4.007000
  END_RES_DEF

  RES_ID          823
  RES_TYPE        LYS
  SPIN_SYSTEM_ID  109
  HETEROGENEITY   100
    N  120.864000
    HN  7.938000
    CA  56.820000
    HA  4.008000
    CB  31.487000
    HB1  1.730000
    HB2  1.567000
    CG  23.226000
    HG1  0.833000
    CD  27.080000
    HD1  1.403000
    CE  42.501000
    HE1  2.569000
    HE2  2.422000
  END_RES_DEF

  RES_ID          824
  RES_TYPE        ILE
  SPIN_SYSTEM_ID  110
  HETEROGENEITY   100
    N  116.928000
    HN  8.101000
    CA  64.530000
    HA  3.818000
    CB  36.990000
    HB  1.746000
    CG1  26.530000
    HG11  1.140000
    HG12  1.073000
    CG2  18.820000
    HG2#  0.654000
    CD1  13.312000
    HD1#  0.541000
  END_RES_DEF

  RES_ID          825
  RES_TYPE        LYS
  SPIN_SYSTEM_ID  111
  HETEROGENEITY   100
    N  122.176000
    HN  7.546000
    CA  59.024000
    HA  4.043000
    CB  32.360000
    HB1  1.879000
    HB2  1.757000
    CG  24.878000
    HG1  1.390000
    HG2  1.302000
    CD  29.284000
    HD1  1.633000
    CE  41.400000
    HE1  2.913000
  END_RES_DEF

  RES_ID          826
  RES_TYPE        GLU
  SPIN_SYSTEM_ID  112
  HETEROGENEITY   100
    N  121.192000
    HN  8.063000
    CA  59.024000
    HA  3.995000
    CB  29.834000
    HB1  2.058000
    CG  36.050000
    HG1  2.342000
    HG2  2.205000
  END_RES_DEF

  RES_ID          827
  RES_TYPE        ALA
  SPIN_SYSTEM_ID  113
  HETEROGENEITY   100
    N  117.748000
    HN  7.620000
    CA  52.410000
    HA  4.291000
    CB  19.920000
    HB#  1.358000
  END_RES_DEF

  RES_ID          828
  RES_TYPE        GLY
  SPIN_SYSTEM_ID  114
  HETEROGENEITY   100
    N  126.767000
    HN  7.744000
    CA  45.902000
    HA1  4.019000
    HA2  3.935000
  END_RES_DEF

  RES_ID          829
  RES_TYPE        LEU
  SPIN_SYSTEM_ID  115
  HETEROGENEITY   100
    N  117.912000
    HN  7.742000
    CA  55.719000
    HA  4.215000
    CB  43.052000
    HB1  1.562000
    CG  27.632000
    HG  1.536000
    CD1  23.776000
    HD1#  0.711000
  END_RES_DEF

  RES_ID          830
  RES_TYPE        ILE
  SPIN_SYSTEM_ID  116
  HETEROGENEITY   100
    N  115.453000
    HN  7.458000
    CA  60.676000
    HA  4.232000
    CB  39.748000
    HB  1.810000
    CG1  27.080000
    HG11  1.314000
    HG12  0.918000
    CG2  17.718000
    HG2#  0.815000
    CD1  13.312000
    HD1#  0.794000
  END_RES_DEF

  RES_ID          831
  RES_TYPE        ASP
  SPIN_SYSTEM_ID  117
  HETEROGENEITY   100
    N  123.488000
    HN  8.270000
    CA  54.620000
    HA  4.571000
    CB  41.400000
    HB1  2.693000
    HB2  2.540000
  END_RES_DEF

  RES_ID          832
  RES_TYPE        LYS
  SPIN_SYSTEM_ID  118
  HETEROGENEITY   100
    N  125.450000
    HN  7.774000
    CA  57.720000
    HA  4.082000
    CB  33.410000
  END_RES_DEF
```

Table 2

Unambiguous NOE-derived Inter-proton Distance Restraints

```
ASSI { 2141}
  (( segid "BrD " and resid 89    and name HN  ))
  (  segid "BrD " and resid 96    and name HD% )
     4 200     4 200     1 300 peak  2141 weight  0 11000E+01 volume  0 36756E+02 ppm1     8 857 ppm2     7 704
ASSI {13261}
  (( segid "BrD " and resid 89    and name HD22))
  (  segid "BrD " and resid 95    and name HE% )
     3 900     3 800     1 600 peak 13261 weight  0 11000E+01 volume  0.50220E+02 ppm1     8 416 ppm2     7.624
ASSI {13271}
  (( segid "BrD " and resid 89    and name HD21))
  (  segid "BrD " and resid 95    and name HE% )
     4 000     4 000     1 500 peak 13271 weight  0 11000E+01 volume  0 43992E+02 ppm1     8 924 ppm2     7 624
ASSI { 8521}
  (( segid "BrD " and resid 46    and name HN  ))
  (  segid "BrD " and resid 47    and name HD% )
     3 500     3.100     2 000 peak  8521 weight  0 11000E+01 volume  0 10017E+03 ppm1     8 562 ppm2     7 960
ASSI {14401}
  (( segid "BrD " and resid 87    and name HN  ))
  (( segid "BrD " and resid 88    and name HB1 ))
     3 700     3 400     1 800 peak 14401 weight  0 11000E+01 volume  0 72183E+02 ppm1     8.572 ppm2     3 532
OR {14401}
  (( segid "BrD " and resid 87    and name HN  ))
  (( segid "BrD " and resid 88    and name HB2 ))
ASSI {15611}
  (( segid "BrD " and resid 32    and name HE1 ))
  (( segid "BrD " and resid 94    and name HG2 ))
     4 500     4.500     1.000 peak 15611 weight  0 11000E+01 volume  0 23846E+02 ppm1    11 082 ppm2     3 143
OR {15611}
  (( segid "BrD " and resid 32    and name HE1 ))
  (( segid "BrD " and resid 94    and name HG1 ))
ASSI {    1}
  (( segid "BrD " and resid 43    and name HN  ))
  (( segid "BrD " and resid 43    and name HA  ))
     2.700     1 800     1 800 peak     1 weight  0 11000E+01 volume  0 52965E+03 ppm1     8 001 ppm2     5.544
ASSI {   11}
  (( segid "BrD " and resid 43    and name HN  ))
  (  segid "BrD " and resid 43    and name HB% )
     2 400     1 400     1 400 peak    11 weight  0 11000E+01 volume  0 93421E+03 ppm1     8 001 ppm2     1 689
ASSI {   21}
  (( segid "BrD " and resid 43    and name HN  ))
  (( segid "BrD " and resid 42    and name HN  ))
     2 200     1.200     1 200 peak    21 weight  0 11000E+01 volume  0 18953E+04 ppm1     8 001 ppm2     7.816
ASSI {   31}
  (( segid "BrD " and resid 42    and name HN  ))
  (( segid "BrD " and resid 41    and name HB  ))
     3.300     2 700     2.200 peak    31 weight  0 11000E+01 volume  0 14380E+03 ppm1     7 822 ppm2     4.900
ASSI {   41}
  (( segid "BrD " and resid 42    and name HN  ))
  (( segid "BrD " and resid 42    and name HA  ))
     2 900     2 100     2 100 peak    41 weight  0 11000E+01 volume  0.30790E+03 ppm1     7 824 ppm2     5 053
ASSI {   51}
  (( segid "BrD " and resid 42    and name HN  ))
  (( segid "BrD " and resid 42    and name HB2 ))
     2 700     1.800     1 800 peak    51 weight  0 11000E+01 volume  0 47343E+03 ppm1     7 821 ppm2     2 613
ASSI {   61}
  (( segid "BrD " and resid 42    and name HN  ))
  (( segid "BrD " and resid 42    and name HG1 ))
     3 200     2.600     2 300 peak    61 weight  0.11000E+01 volume  0 16643E+03 ppm1     7 822 ppm2     2 899
ASSI {   71}
  (( segid "BrD " and resid 42    and name HN  ))
  (( segid "BrD " and resid 42    and name HB1 ))
     3 400     2 900     2.100 peak    71 weight  0.11000E+01 volume  0 13090E+03 ppm1     7 821 ppm2     2 790
ASSI {   91}
  (( segid "BrD " and resid 99    and name HN  ))
  (  segid "BrD " and resid 99    and name HB% )
     2 400     1 400     1 400 peak    91 weight  0 11000E+01 volume  0 90687E+03 ppm1     8 936 ppm2     2.208
ASSI {  101}
  (( segid "BrD " and resid 99    and name HN  ))
  (( segid "BrD " and resid 99    and name HA  ))
     2.800     2 000     2.000 peak   101 weight  0 11000E+01 volume  0 42952E+03 ppm1     8 936 ppm2     4 441
ASSI {  121}
  (( segid "BrD " and resid 99    and name HN  ))
  (( segid "BrD " and resid 98    and name HN  ))
     2.700     1 800     1 800 peak   121 weight  0 11000E+01 volume  0 45502E+03 ppm1     8.936 ppm2     9 112
ASSI {  131}
  (( segid "BrD " and resid 98    and name HN  ))
  (( segid "BrD " and resid 98    and name HA  ))
     2 500     1 600     1 600 peak   131 weight  0 11000E+01 volume  0 72592E+03 ppm1     9.125 ppm2     4 811
ASSI {  141}
  (( segid "BrD " and resid 98    and name HN  ))
  (( segid "BrD " and resid 98    and name HB1 ))
     3 300     2 700     2.200 peak   141 weight  0 11000E+01 volume  0 15487E+03 ppm1     9 125 ppm2     4.010
ASSI {  151}
  (( segid "BrD " and resid 98    and name HN  ))
  (( segid "BrD " and resid 98    and name HB2 ))
     2.400     1 400     1 400 peak   151 weight  0 11000E+01 volume  0 95273E+03 ppm1     9 125 ppm2     3 656
ASSI {  171}
  (( segid "BrD " and resid 30    and name HN  ))
  (( segid "BrD " and resid 30    and name HA  ))
     3 100     2.400     2 400 peak   171 weight  0 11000E+01 volume  0 20628E+03 ppm1    12 275 ppm2     5 451
ASSI {  181}
  (( segid "BrD " and resid 30    and name HN  ))
  (( segid "BrD " and resid 30    and name HB1 ))
     3 200     2 600     2.300 peak   181 weight  0 11000E+01 volume  0 16806E+03 ppm1    12 275 ppm2     4.939
ASSI {  191}
  (( segid "BrD " and resid 30    and name HN  ))
  (( segid "BrD " and resid 30    and name HB2 ))
     2 800     2 000     2 000 peak   191 weight  0.11000E+01 volume  0 40863E+03 ppm1    12 275 ppm2     4 538
ASSI {  201}
  (( segid "BrD " and resid 30    and name HN  ))
  (( segid "BrD " and resid 29    and name HN  ))
     3 300     2 700     2 200 peak   201 weight  0.11000E+01 volume  0 15134E+03 ppm1    12 275 ppm2     9 150
ASSI {  211}
  (( segid "BrD " and resid 29    and name HN  ))
  (( segid "BrD " and resid 29    and name HA  ))
     2 700     1 800     1 800 peak   211 weight  0 11000E+01 volume  0 44648E+03 ppm1     9 151 ppm2     4 818
ASSI {  221}
  (( segid "BrD " and resid 29    and name HN  ))
  (( segid "BrD " and resid 29    and name HB1 ))
     2 800     2 000     2 000 peak   221 weight  0.11000E+01 volume  0 39478E+03 ppm1     9 152 ppm2     2 712
ASSI {  231}
  (( segid "BrD " and resid 31    and name HN  ))
  (( segid "BrD " and resid 29    and name HA  ))
     3 400     2 900     2 100 peak   231 weight  0.11000E+01 volume  0 12405E+03 ppm1     8 479 ppm2     4 816
ASSI {  241}
  (( segid "BrD " and resid 31    and name HN  ))
  (( segid "BrD " and resid 31    and name HA  ))
     3 300     2 700     2 200 peak   241 weight  0.11000E+01 volume  0 13933E+03 ppm1     8 479 ppm2     5 003
ASSI {  251}
  (( segid "BrD " and resid 31    and name HN  ))
  (  segid "BrD " and resid 31    and name HB% )
     2 400     1 400     1 400 peak   251 weight  0 11000E+01 volume  0 88455E+03 ppm1     8 480 ppm2     2 307
ASSI {  271}
  (( segid "BrD " and resid 28    and name HN  ))
  (( segid "BrD " and resid 28    and name HB2 ))
     2 500     1 600     1.600 peak   271 weight  0 11000E+01 volume  0 82952E+03 ppm1     8 166 ppm2     3 409
ASSI {  281}
  (( segid "BrD " and resid 28    and name HN  ))
  (( segid "BrD " and resid 28    and name HB1 ))
     2 500     1 600     1 600 peak   281 weight  0 11000E+01 volume  0 71832E+03 ppm1     8 166 ppm2     3 596
ASSI {  291}
  (( segid "BrD " and resid 28    and name HN  ))
  (( segid "BrD " and resid 28    and name HA  ))
     2 700     1.800     1.800 peak   291 weight  0 11000E+01 volume  0 53058E+03 ppm1     8 165 ppm2     4 598
ASSI {  301}
  (( segid "BrD " and resid 28    and name HN  ))
  (( segid "BrD " and resid 29    and name HN  ))
     3 400     2 900     2 100 peak   301 weight  0 11000E+01 volume  0 11688E+03 ppm1     8 166 ppm2     9 164
ASSI {  321}
  (( segid "BrD " and resid 32    and name HN  ))
  (( segid "BrD " and resid 32    and name HA  ))
     2.600     1 700     1 700 peak   321 weight  0 11000E+01 volume  0 66621E+03 ppm1     7 739 ppm2     4 977
ASSI {  331}
  (( segid "BrD " and resid 32    and name HN  ))
  (( segid "BrD " and resid 32    and name HB1 ))
     2.900     2 100     2 100 peak   331 weight  0.11000E+01 volume  0 30872E+03 ppm1     7 740 ppm2     4.201
ASSI {  341}
  (( segid "BrD " and resid 32    and name HN  ))
  (( segid "BrD " and resid 32    and name HB2 ))
     2.600     1 700     1 700 peak   341 weight  0 11000E+01 volume  0 59972E+03 ppm1     7 739 ppm2     3.958
ASSI {  351}
  (( segid "BrD " and resid 30    and name HN  ))
  (( segid "BrD " and resid 31    and name HN  ))
     2.800     2.000     2 000 peak   351 weight  0 11000E+01 volume  0 41861E+03 ppm1    12 275 ppm2     8 477
ASSI {  361}
  (( segid "BrD " and resid 105   and name HN  ))
  (( segid "BrD " and resid 105   and name HA  ))
     3.100     2.400     2 400 peak   361 weight  0 11000E+01 volume  0 22043E+03 ppm1     8 488 ppm2     4 934
ASSI {  371}
  (( segid "BrD " and resid 105   and name HN  ))
  (( segid "BrD " and resid 105   and name HB1 ))
     2.800     2.000     2.000 peak   371 weight  0.11000E+01 volume  0 42542E+03 ppm1     8 487 ppm2     3 740
ASSI {  401}
  (( segid "BrD " and resid 106   and name HN  ))
  (( segid "BrD " and resid 105   and name HN  ))
     2 700     1.800     1.800 peak   401 weight  0.11000E+01 volume  0.44987E+03 ppm1     9 740 ppm2     8.476
ASSI {  411}
  (( segid "BrD " and resid 106   and name HN  ))
  (( segid "BrD " and resid 106   and name HA  ))
     2 600     1 700     1 700 peak   411 weight  0.11000E+01 volume  0 55394E+03 ppm1     9 740 ppm2     4 566
ASSI {  421}
  (( segid "BrD " and resid 106   and name HN  ))
  (( segid "BrD " and resid 106   and name HB1 ))
     2 500     1.600     1.600 peak   421 weight  0 11000E+01 volume  0 71565E+03 ppm1     9 740 ppm2     3.895
ASSI {  431}
  (( segid "BrD " and resid 106   and name HN  ))
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  (( segid "BrD " and resid 106  and name HB2 ))
     2.300     1.300     1.300 peak   431 weight  0.11000E+01 volume  0.11998E+04 ppm1     9.740 ppm2     3.674
ASSI {  451}
  (( segid "BrD " and resid 107  and name HN  ))
  (( segid "BrD " and resid 106  and name HN  ))
     2 900     2.100     2 100 peak   451 weight  0 11000E+01 volume  0.34881E+03 ppm1     8 981 ppm2     9 733
ASSI {  461}
  (( segid "BrD " and resid 107  and name HN  ))
  (  segid "BrD " and resid 107  and name HD% )
     3 500     3 100     2 000 peak   461 weight  0 11000E+01 volume  0 11255E+03 ppm1     8 980 ppm2     7.783
ASSI {  471}
  (( segid "BrD " and resid 107  and name HN  ))
  (( segid "BrD " and resid 107  and name HA  ))
     2 600     1 700     1 700 peak   471 weight  0.11000E+01 volume  0 57631E+03 ppm1     8 981 ppm2     4 443
ASSI {  481}
  (( segid "BrD " and resid 107  and name HN  ))
  (( segid "BrD " and resid 107  and name HB1 ))
     3 200     2 600     2 300 peak   481 weight  0 11000E+01 volume  0 16715E+03 ppm1     8 980 ppm2     3 671
ASSI {  501}
  (( segid "BrD " and resid 108  and name HN  ))
  (( segid "BrD " and resid 107  and name HN  ))
     2 600     1 700     1 700 peak   501 weight  0.11000E+01 volume  0.57313E+03 ppm1     8 529 ppm2     8 966
ASSI {  511}
  (( segid "BrD " and resid 108  and name HN  ))
  (( segid "BrD " and resid 108  and name HA  ))
     2 700     1 800     1.800 peak   511 weight  0 11000E+01 volume  0 52916E+03 ppm1     8 526 ppm2     4 811
ASSI {  521}
  (( segid "BrD " and resid 108  and name HN  ))
  (( segid "BrD " and resid 108  and name HB1 ))
     2 400     1 400     1 400 peak   521 weight  0 11000E+01 volume  0 97994E+03 ppm1     8 526 ppm2     4 583
ASSI {  531}
  (( segid "BrD " and resid 109  and name HN  ))
  (( segid "BrD " and resid 109  and name HA  ))
     2 300     1 300     1 300 peak   531 weight  0 11000E+01 volume  0 11922E+04 ppm1     8 572 ppm2     4 615
ASSI {  541}
  (( segid "BrD " and resid 110  and name HN  ))
  (( segid "BrD " and resid 109  and name HB2 ))
     2 900     2 100     2 100 peak   541 weight  0 11000E+01 volume  0 32815E+03 ppm1     8 714 ppm2     2 174
ASSI {  551}
  (( segid "BrD " and resid 110  and name HN  ))
  (( segid "BrD " and resid 110  and name HA  ))
     2 800     2 000     2 000 peak   551 weight  0 11000E+01 volume  0 43619E+03 ppm1     8 714 ppm2     4 451
ASSI {  561}
  (( segid "BrD " and resid 110  and name HN  ))
  (( segid "BrD " and resid 110  and name HB  ))
     2 500     1 600     1 600 peak   561 weight  0 11000E+01 volume  0 77600E+03 ppm1     8 714 ppm2     2 352
ASSI {  581}
  (( segid "BrD " and resid 109  and name HN  ))
  (( segid "BrD " and resid 110  and name HN  ))
     2 800     2 000     2.000 peak   581 weight  0 11000E+01 volume  0 41482E+03 ppm1     8 572 ppm2     8 705
ASSI {  591}
  (( segid "BrD " and resid 111  and name HN  ))
  (( segid "BrD " and resid 108  and name HA  ))
     3 200     2 600     2.300 peak   591 weight  0.11000E+01 volume  0 17690E+03 ppm1     8 168 ppm2     4 807
ASSI {  601}
  (( segid "BrD " and resid 111  and name HN  ))
  (( segid "BrD " and resid 111  and name HA  ))
     2 500     1 600     1 600 peak   601 weight  0 11000E+01 volume  0 71549E+03 ppm1     8 168 ppm2     4 650
ASSI {  621}
  (( segid "BrD " and resid 110  and name HN  ))
  (( segid "BrD " and resid 111  and name HN  ))
     2 800     2 000     2 000 peak   621 weight  0.11000E+01 volume  0 38661E+03 ppm1     8 714 ppm2     8 153
ASSI {  631}
  (( segid "BrD " and resid 112  and name HN  ))
  (( segid "BrD " and resid 112  and name HA  ))
     2 300     1 300     1 300 peak   631 weight  0 11000E+01 volume  0 13944E+04 ppm1     8 667 ppm2     4 607
ASSI {  641}
  (( segid "BrD " and resid 112  and name HN  ))
  (( segid "BrD " and resid 112  and name HG1 ))
     3 400     2 900     2 100 peak   641 weight  0 11000E+01 volume  0 12114E+03 ppm1     8 668 ppm2     2 956
ASSI {  651}
  (( segid "BrD " and resid 112  and name HN  ))
  (( segid "BrD " and resid 112  and name HG2 ))
     3 500     3 100     2 000 peak   651 weight  0 11000E+01 volume  0 96511E+02 ppm1     8 668 ppm2     2 818
ASSI {  661}
  (( segid "BrD " and resid 112  and name HN  ))
  (( segid "BrD " and resid 112  and name HB1 ))
     2.200     1 200     1 200 peak   661 weight  0.11000E+01 volume  0 15417E+04 ppm1     8 668 ppm2     2 667
ASSI {  671}
  (( segid "BrD " and resid 113  and name HN  ))
  (( segid "BrD " and resid 113  and name HA  ))
     2 800     2 000     2 000 peak   671 weight  0 11000E+01 volume  0 42878E+03 ppm1     8 217 ppm2     4 904
ASSI {  681}
  (( segid "BrD " and resid 113  and name HN  ))
  (  segid "BrD " and resid 113  and name HB% )
     2 400     1 400     1 400 peak   681 weight  0 11000E+01 volume  0 99017E+03 ppm1     8 219 ppm2     1.967
ASSI {  701}
  (( segid "BrD " and resid 114  and name HN  ))
  (( segid "BrD " and resid 114  and name HA1 ))
     2.800     2 000     2 000 peak   701 weight  0.11000E+01 volume  0 42782E+03 ppm1     8 376 ppm2     4 619
ASSI {  721}
  (( segid "BrD " and resid 113  and name HN  ))
  (( segid "BrD " and resid 114  and name HN  ))
     2 500     1.600     1 600 peak   721 weight  0.11000E+01 volume  0 73856E+03 ppm1     8.219 ppm2     8 351
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ASSI {  741}
  (( segid "BrD " and resid 100  and name HN  ))
  (( segid "BrD " and resid 100  and name HA  ))
     2.700     1 800     1 800 peak   741 weight  0 11000E+01 volume  0 49224E+03 ppm1     8 669 ppm2     4 938
ASSI {  751}
  (( segid "BrD " and resid 100  and name HN  ))
  (( segid "BrD " and resid 100  and name HB2 ))
     2 400     1 400     1 400 peak   751 weight  0 11000E+01 volume  0.10916E+04 ppm1     8.669 ppm2     3 422
ASSI {  771}
  (( segid "BrD " and resid 99   and name HN  ))
  (( segid "BrD " and resid 100  and name HN  ))
     2 500     1.600     1.600 peak   771 weight  0 11000E+01 volume  0 76441E+03 ppm1     8 936 ppm2     8 664
ASSI {  791}
  (( segid "BrD " and resid 97   and name HN  ))
  (( segid "BrD " and resid 97   and name HA  ))
     2 600     1 700     1 700 peak   791 weight  0 11000E+01 volume  0 58097E+03 ppm1     8.676 ppm2     4 809
ASSI {  811}
  (( segid "BrD " and resid 97   and name HN  ))
  (( segid "BrD " and resid 98   and name HN  ))
     3 000     2 200     2 200 peak   811 weight  0 11000E+01 volume  0 25513E+03 ppm1     8 672 ppm2     9 124
ASSI {  841}
  (( segid "BrD " and resid 96   and name HN  ))
  (( segid "BrD " and resid 96   and name HA  ))
     2 600     1 700     1 700 peak   841 weight  0 11000E+01 volume  0 65098E+03 ppm1     7 977 ppm2     4 433
ASSI {  851}
  (( segid "BrD " and resid 96   and name HN  ))
  (( segid "BrD " and resid 96   and name HB1 ))
     2 800     2 000     2 000 peak   851 weight  0 11000E+01 volume  0 42091E+03 ppm1     7 976 ppm2     3 995
ASSI {  861}
  (( segid "BrD " and resid 96   and name HN  ))
  (( segid "BrD " and resid 96   and name HB2 ))
     2 600     1 700     1 700 peak   861 weight  0 11000E+01 volume  0 56648E+03 ppm1     7 979 ppm2     3 112
ASSI {  871}
  (( segid "BrD " and resid 96   and name HN  ))
  (( segid "BrD " and resid 97   and name HN  ))
     2 600     1 700     1 700 peak   871 weight  0 11000E+01 volume  0 67038E+03 ppm1     7 979 ppm2     8 678
ASSI {  891}
  (( segid "BrD " and resid 95   and name HN  ))
  (( segid "BrD " and resid 95   and name HA  ))
     3 100     2 400     2 400 peak   891 weight  0 11000E+01 volume  0 22376E+03 ppm1     8 669 ppm2     4 443
ASSI {  901}
  (( segid "BrD " and resid 95   and name HN  ))
  (( segid "BrD " and resid 95   and name HB1 ))
     2 800     2 000     2 000 peak   901 weight  0 11000E+01 volume  0 37061E+03 ppm1     8 669 ppm2     3 598
ASSI {  911}
  (( segid "BrD " and resid 95   and name HN  ))
  (( segid "BrD " and resid 95   and name HB2 ))
     2 700     1 800     1 800 peak   911 weight  0 11000E+01 volume  0 54351E+03 ppm1     8 669 ppm2     3.346
ASSI {  921}
  (( segid "BrD " and resid 94   and name HN  ))
  (( segid "BrD " and resid 94   and name HA  ))
     3 300     2 700     2 200 peak   921 weight  0 11000E+01 volume  0 13528E+03 ppm1     9 679 ppm2     4.846
ASSI {  941}
  (( segid "BrD " and resid 94   and name HN  ))
  (( segid "BrD " and resid 95   and name HN  ))
     3.500     3 100     2 000 peak   941 weight  0 11000E+01 volume  0 95054E+02 ppm1     9.679 ppm2     8 670
ASSI {  971}
  (( segid "BrD " and resid 93   and name HN  ))
  (( segid "BrD " and resid 93   and name HA  ))
     3 200     2 600     2 300 peak   971 weight  0 11000E+01 volume  0 16612E+03 ppm1     8 713 ppm2     5.037
ASSI {  981}
  (( segid "BrD " and resid 93   and name HN  ))
  (( segid "BrD " and resid 93   and name HB2 ))
     3 300     2 700     2 200 peak   981 weight  0 11000E+01 volume  0 15761E+03 ppm1     8 713 ppm2     4 753
ASSI { 1001}
  (( segid "BrD " and resid 92   and name HN  ))
  (( segid "BrD " and resid 92   and name HA  ))
     2 500     1 600     1 600 peak  1001 weight  0 11000E+01 volume  0 71435E+03 ppm1     8 873 ppm2     4.802
ASSI { 1011}
  (( segid "BrD " and resid 92   and name HN  ))
  (( segid "BrD " and resid 93   and name HN  ))
     2 500     1 600     1 600 peak  1011 weight  0 11000E+01 volume  0 69883E+03 ppm1     8 871 ppm2     8 719
ASSI { 1031}
  (( segid "BrD " and resid 76   and name HN  ))
  (( segid "BrD " and resid 76   and name HA  ))
     2 500     1 600     1 600 peak  1031 weight  0 11000E+01 volume  0 86678E+03 ppm1     8 611 ppm2     4 688
ASSI { 1041}
  (( segid "BrD " and resid 76   and name HN  ))
  (  segid "BrD " and resid 76   and name HB% )
     2 200     1 200     1 200 peak  1041 weight  0.11000E+01 volume  0 16592E+04 ppm1     8 612 ppm2     2 102
ASSI { 1061}
  (( segid "BrD " and resid 77   and name HN  ))
  (( segid "BrD " and resid 77   and name HA  ))
     2 700     1 800     1 800 peak  1061 weight  0.11000E+01 volume  0 53554E+03 ppm1     7 996 ppm2     4 980
ASSI { 1071}
  (( segid "BrD " and resid 77   and name HN  ))
  (( segid "BrD " and resid 77   and name HB1 ))
     2 100     1 100     1 100 peak  1071 weight  0 11000E+01 volume  0 22098E+04 ppm1     7 996 ppm2     3 337
ASSI { 1091}
  (( segid "BrD " and resid 76   and name HN  ))
  (( segid "BrD " and resid 77   and name HN  ))
     2.600     1 700     1 700 peak  1091 weight  0 11000E+01 volume  0.57823E+03 ppm1     8 612 ppm2     7 983
ASSI { 1111}
  (( segid "BrD " and resid 75   and name HN  ))
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(( segid "BrD " and resid 75   and name HA  ))
   2.800     2.000     2.000 peak  1111 weight  0.11000E+01 volume  0.40919E+03 ppm1     9.106 ppm2     4 527
ASSI { 1121}
 (( segid "BrD " and resid 75   and name HN  ))
 (( segid "BrD " and resid 75   and name HG1 ))
   2.600     1 700     1 700 peak  1121 weight  0 11000E+01 volume  0 66185E+03 ppm1     9 106 ppm2     3 549
ASSI { 1131}
 (( segid "BrD " and resid 75   and name HN  ))
 (( segid "BrD " and resid 75   and name HG2 ))
   2 900     2 100     2 100 peak  1131 weight  0 11000E+01 volume  0 30957E+03 ppm1     9.106 ppm2     3 221
ASSI { 1141}
 (( segid "BrD " and resid 75   and name HN  ))
 (( segid "BrD " and resid 75   and name HB1 ))
   3 100     2.400     2 400 peak  1141 weight  0 11000E+01 volume  0 19539E+03 ppm1     9 106 ppm2     2 919
ASSI { 1151}
 (( segid "BrD " and resid 75   and name HN  ))
 (( segid "BrD " and resid 75   and name HB2 ))
   2 500     1 600     1 600 peak  1151 weight  0 11000E+01 volume  0 72202E+03 ppm1     9 106 ppm2     2 816
ASSI { 1171}
 (( segid "BrD " and resid 76   and name HN  ))
 (( segid "BrD " and resid 75   and name HN  ))
   2 700     1 800     1.800 peak  1171 weight  0 11000E+01 volume  0 51792E+03 ppm1     8.613 ppm2     9.085
ASSI { 1181}
 (( segid "BrD " and resid 74   and name HN  ))
 (  segid "BrD " and resid 74   and name HD% )
   3 000     2 200     2 200 peak  1181 weight  0 11000E+01 volume  0 24258E+03 ppm1     7 536 ppm2     7 004
ASSI { 1191}
 (( segid "BrD " and resid 74   and name HN  ))
 (( segid "BrD " and resid 74   and name HA  ))
   3 000     2 200     2 200 peak  1191 weight  0 11000E+01 volume  0 27313E+03 ppm1     7 536 ppm2     4 368
ASSI { 1201}
 (( segid "BrD " and resid 74   and name HN  ))
 (( segid "BrD " and resid 74   and name HB1 ))
   2 800     2 000     2 000 peak  1201 weight  0 11000E+01 volume  0.42552E+03 ppm1     7.535 ppm2     3 552
ASSI { 1211}
 (( segid "BrD " and resid 74   and name HN  ))
 (( segid "BrD " and resid 74   and name HB2 ))
   2 700     1 800     1 800 peak  1211 weight  0 11000E+01 volume  0 47386E+03 ppm1     7 536 ppm2     2 983
ASSI { 1231}
 (( segid "BrD " and resid 75   and name HN  ))
 (( segid "BrD " and resid 74   and name HN  ))
   2 800     2 000     2 000 peak  1231 weight  0 11000E+01 volume  0.42446E+03 ppm1     9 105 ppm2     7 535
ASSI { 1241}
 (( segid "BrD " and resid 70   and name HN  ))
 (( segid "BrD " and resid 70   and name HA  ))
   2 500     1 600     1 600 peak  1241 weight  0 11000E+01 volume  0 78559E+03 ppm1     8 040 ppm2     5 348
ASSI { 1251}
 (( segid "BrD " and resid 70   and name HN  ))
 (( segid "BrD " and resid 70   and name HB2 ))
   2 900     2 100     2 100 peak  1251 weight  0 11000E+01 volume  0 29096E+03 ppm1     8 039 ppm2     4 357
ASSI { 1261}
 (( segid "BrD " and resid 69   and name HN  ))
 (( segid "BrD " and resid 69   and name HA  ))
   2 800     2 000     2 000 peak  1261 weight  0 11000E+01 volume  0 43807E+03 ppm1     8 306 ppm2     4.690
ASSI { 1271}
 (( segid "BrD " and resid 69   and name HN  ))
 (( segid "BrD " and resid 69   and name HB  ))
   3 300     2 700     2 200 peak  1271 weight  0 11000E+01 volume  0 13733E+03 ppm1     8 306 ppm2     2 921
ASSI { 1281}
 (( segid "BrD " and resid 69   and name HN  ))
 (  segid "BrD " and resid 69   and name HG1%)
   2 800     2 000     2 000 peak  1281 weight  0 11000E+01 volume  0 40608E+03 ppm1     8 306 ppm2     1 549
ASSI { 1291}
 (( segid "BrD " and resid 69   and name HN  ))
 (  segid "BrD " and resid 69   and name HG2%)
   3 000     2 200     2 200 peak  1291 weight  0 11000E+01 volume  0 24335E+03 ppm1     8.306 ppm2     1 430
ASSI { 1301}
 (( segid "BrD " and resid 69   and name HN  ))
 (( segid "BrD " and resid 70   and name HN  ))
   2 800     2 000     2 000 peak  1301 weight  0 11000E+01 volume  0 40402E+03 ppm1     8 306 ppm2     8.022
ASSI { 1321}
 (( segid "BrD " and resid 68   and name HN  ))
 (  segid "BrD " and resid 68   and name HD% )
   2 900     2 100     2 100 peak  1321 weight  0 11000E+01 volume  0 34716E+03 ppm1     8 626 ppm2     7 778
ASSI { 1331}
 (( segid "BrD " and resid 68   and name HN  ))
 (( segid "BrD " and resid 68   and name HA  ))
   3 200     2.600     2 300 peak  1331 weight  0.11000E+01 volume  0.16288E+03 ppm1     8 626 ppm2     5 142
ASSI { 1341}
 (( segid "BrD " and resid 68   and name HN  ))
 (( segid "BrD " and resid 68   and name HB1 ))
   3 000     2 200     2.200 peak  1341 weight  0 11000E+01 volume  0 26781E+03 ppm1     8 625 ppm2     3 669
ASSI { 1351}
 (( segid "BrD " and resid 68   and name HN  ))
 (( segid "BrD " and resid 68   and name HB2 ))
   2 700     1 800     1 800 peak  1351 weight  0.11000E+01 volume  0.52551E+03 ppm1     8 627 ppm2     3.516
ASSI { 1361}
 (( segid "BrD " and resid 68   and name HN  ))
 (( segid "BrD " and resid 69   and name HN  ))
   3 500     3.100     2 000 peak  1361 weight  0 11000E+01 volume  0 11066E+03 ppm1     8.622 ppm2     8 304
ASSI { 1381}
 (( segid "BrD " and resid 67   and name HN  ))
 (  segid "BrD " and resid 67   and name HD% )
   3 100     2 400     2 400 peak  1381 weight  0 11000E+01 volume  0.20078E+03 ppm1     8 832 ppm2     6 888
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ASSI { 1391}
 (( segid "BrD " and resid 67   and name HN  ))
 (( segid "BrD " and resid 67   and name HA  ))
   2 800     2 000     2 000 peak  1391 weight  0 11000E+01 volume  0 36081E+03 ppm1     8 832 ppm2     4.671
ASSI { 1401}
 (( segid "BrD " and resid 67   and name HN  ))
 (( segid "BrD " and resid 67   and name HB1 ))
   2 900     2 100     2 100 peak  1401 weight  0 11000E+01 volume  0 31437E+03 ppm1     8 832 ppm2     3 549
ASSI { 1411}
 (( segid "BrD " and resid 67   and name HN  ))
 (( segid "BrD " and resid 67   and name HB2 ))
   2 400     1 400     1 400 peak  1411 weight  0 11000E+01 volume  0 92322E+03 ppm1     8 833 ppm2     2 661
ASSI { 1431}
 (( segid "BrD " and resid 68   and name HN  ))
 (( segid "BrD " and resid 67   and name HN  ))
   2 500     1 600     1 600 peak  1431 weight  0 11000E+01 volume  0 76621E+03 ppm1     8 622 ppm2     8 829
ASSI { 1441}
 (( segid "BrD " and resid 68   and name HN  ))
 (  segid "BrD " and resid 67   and name HD% )
   3 200     2 600     2 300 peak  1441 weight  0 11000E+01 volume  0 16656E+03 ppm1     8 626 ppm2     6 892
ASSI { 1451}
 (( segid "BrD " and resid 66   and name HN  ))
 (( segid "BrD " and resid 66   and name HA  ))
   2 200     1 200     1 200 peak  1451 weight  0.11000E+01 volume  0 17604E+04 ppm1     8.763 ppm2     5 001
ASSI { 1461}
 (( segid "BrD " and resid 65   and name HN  ))
 (( segid "BrD " and resid 65   and name HA  ))
   2 500     1 600     1 600 peak  1461 weight  0 11000E+01 volume  0 81596E+03 ppm1     8 564 ppm2     5 375
ASSI { 1471}
 (( segid "BrD " and resid 65   and name HN  ))
 (( segid "BrD " and resid 65   and name HB1 ))
   2.600     1 700     1 700 peak  1471 weight  0 11000E+01 volume  0.66517E+03 ppm1     8 566 ppm2     3 627
ASSI { 1481}
 (( segid "BrD " and resid 65   and name HN  ))
 (( segid "BrD " and resid 65   and name HB2 ))
   2 400     1.400     1 400 peak  1481 weight  0 11000E+01 volume  0 98393E+03 ppm1     8 564 ppm2     3 382
ASSI { 1491}
 (( segid "BrD " and resid 65   and name HN  ))
 (( segid "BrD " and resid 64   and name HB1 ))
   2 400     1 400     1 400 peak  1491 weight  0 11000E+01 volume  0 10161E+04 ppm1     8 565 ppm2     2 659
ASSI { 1501}
 (( segid "BrD " and resid 65   and name HN  ))
 (( segid "BrD " and resid 66   and name HN  ))
   2 300     1 300     1 300 peak  1501 weight  0 11000E+01 volume  0 13482E+04 ppm1     8 565 ppm2     8 765
ASSI { 1521}
 (( segid "BrD " and resid 20   and name HN  ))
 (( segid "BrD " and resid 16   and name HA  ))
   2 700     1 800     1 800 peak  1521 weight  0.11000E+01 volume  0 44067E+03 ppm1     8 146 ppm2     4 527
ASSI { 1531}
 (( segid "BrD " and resid 20   and name HN  ))
 (( segid "BrD " and resid 20   and name HA  ))
   2 500     1 600     1 600 peak  1531 weight  0 11000E+01 volume  0 84286E+03 ppm1     8 146 ppm2     4 895
ASSI { 1541}
 (( segid "BrD " and resid 20   and name HN  ))
 (( segid "BrD " and resid 20   and name HB1 ))
   2 300     1.300     1 300 peak  1541 weight  0.11000E+01 volume  0 13472E+04 ppm1     8 147 ppm2     4.669
ASSI { 1561}
 (( segid "BrD " and resid 21   and name HN  ))
 (( segid "BrD " and resid 21   and name HA  ))
   2 900     2 100     2 100 peak  1561 weight  0 11000E+01 volume  0 31054E+03 ppm1     8.546 ppm2     4 367
ASSI { 1571}
 (( segid "BrD " and resid 101  and name HN  ))
 (( segid "BrD " and resid 101  and name HB  ))
   2 700     1 800     1.800 peak  1571 weight  0 11000E+01 volume  0.51528E+03 ppm1     8 514 ppm2     2 538
ASSI { 1581}
 (( segid "BrD " and resid 22   and name HN  ))
 (( segid "BrD " and resid 22   and name HA  ))
   2 700     1 800     1 800 peak  1581 weight  0 11000E+01 volume  0 45405E+03 ppm1     9 456 ppm2     4 712
ASSI { 1591}
 (( segid "BrD " and resid 23   and name HN  ))
 (( segid "BrD " and resid 21   and name HB  ))
   3.300     2 700     2.200 peak  1591 weight  0 11000E+01 volume  0 13959E+03 ppm1     9 122 ppm2     2 486
ASSI { 1601}
 (( segid "BrD " and resid 23   and name HN  ))
 (( segid "BrD " and resid 23   and name HA  ))
   2 600     1 700     1 700 peak  1601 weight  0 11000E+01 volume  0.61098E+03 ppm1     9 118 ppm2     4.645
ASSI { 1611}
 (( segid "BrD " and resid 23   and name HN  ))
 (( segid "BrD " and resid 23   and name HG1 ))
   3.400     2 900     2 100 peak  1611 weight  0 11000E+01 volume  0 11565E+03 ppm1     9 119 ppm2     3 143
ASSI { 1621}
 (( segid "BrD " and resid 23   and name HN  ))
 (( segid "BrD " and resid 23   and name HB1 ))
   2.900     2 100     2.100 peak  1621 weight  0 11000E+01 volume  0.34650E+03 ppm1     9 118 ppm2     2.939
ASSI { 1641}
 (( segid "BrD " and resid 22   and name HN  ))
 (( segid "BrD " and resid 23   and name HN  ))
   2 600     1 700     1.700 peak  1641 weight  0.11000E+01 volume  0.57061E+03 ppm1     9 456 ppm2     9 123
ASSI { 1651}
 (( segid "BrD " and resid 15   and name HN  ))
 (  segid "BrD " and resid 15   and name HD% )
   3 100     2.400     2 400 peak  1651 weight  0 11000E+01 volume  0 20888E+03 ppm1     8 598 ppm2     7 663
ASSI { 1661}
 (( segid "BrD " and resid 24   and name HN  ))
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  (( segid "BrD " and resid 24   and name HA  ))
    2.800     2.000     2.000 peak  1661 weight  0.11000E+01 volume  0.43492E+03 ppm1     8.661 ppm2     4.775
ASSI { 1671}
  (( segid "BrD " and resid 24   and name HN  ))
  (( segid "BrD " and resid 24   and name HG1 ))
    2 800     2 000     2 000 peak  1671 weight  0 11000E+01 volume  0 42365E+03 ppm1     8.660 ppm2     3 454
ASSI { 1681}
  (( segid "BrD " and resid 24   and name HN  ))
  (( segid "BrD " and resid 24   and name HB1 ))
    2.800     2 000     2 000 peak  1681 weight  0.11000E+01 volume  0 37096E+03 ppm1     8 654 ppm2     3.089
ASSI { 1691}
  (( segid "BrD " and resid 24   and name HN  ))
  (( segid "BrD " and resid 23   and name HN  ))
    2 300     1 300     1.300 peak  1691 weight  0 11000E+01 volume  0.12196E+04 ppm1     8 659 ppm2     9 112
ASSI { 1711}
  (( segid "BrD " and resid 25   and name HN  ))
  (( segid "BrD " and resid 27   and name HN  ))
    3 600     3.200     1.900 peak  1711 weight  0 11000E+01 volume  0 81722E+02 ppm1     9 134 ppm2     8 155
ASSI { 1721}
  (( segid "BrD " and resid 25   and name HN  ))
  (( segid "BrD " and resid 25   and name HA  ))
    3 200     2 600     2 300 peak  1721 weight  0 11000E+01 volume  0 16529E+03 ppm1     9.134 ppm2     4.443
ASSI { 1731}
  (( segid "BrD " and resid 25   and name HN  ))
  (( segid "BrD " and resid 25   and name HB  ))
    2 800     2 000     2 000 peak  1731 weight  0 11000E+01 volume  0 35564E+03 ppm1     9 132 ppm2     2 984
ASSI { 1741}
  (( segid "BrD " and resid 25   and name HN  ))
  (  segid "BrD " and resid 25   and name HG1%)
    2 600     1 700     1.700 peak  1741 weight  0 11000E+01 volume  0 61322E+03 ppm1     9 133 ppm2     1 799
ASSI { 1751}
  (( segid "BrD " and resid 25   and name HN  ))
  (  segid "BrD " and resid 25   and name HG2%)
    2 800     2 000     2 000 peak  1751 weight  0 11000E+01 volume  0 35918E+03 ppm1     9 133 ppm2     1 627
ASSI { 1771}
  (( segid "BrD " and resid 24   and name HN  ))
  (( segid "BrD " and resid 25   and name HN  ))
    2 400     1.400     1.400 peak  1771 weight  0 11000E+01 volume  0 91823E+03 ppm1     8 661 ppm2     9.133
ASSI { 1791}
  (( segid "BrD " and resid 26   and name HN  ))
  (( segid "BrD " and resid 26   and name HA  ))
    3 000     2 200     2 200 peak  1791 weight  0 11000E+01 volume  0.24501E+03 ppm1     9 196 ppm2     4 488
ASSI { 1801}
  (( segid "BrD " and resid 27   and name HN  ))
  (( segid "BrD " and resid 26   and name HB1 ))
    2 700     1 800     1 800 peak  1801 weight  0 11000E+01 volume  0 50197E+03 ppm1     8 169 ppm2     2 480
ASSI { 1811}
  (( segid "BrD " and resid 27   and name HN  ))
  (( segid "BrD " and resid 27   and name HA  ))
    2 700     1 800     1 800 peak  1811 weight  0 11000E+01 volume  0 49453E+03 ppm1     8 170 ppm2     5 055
ASSI { 1821}
  (( segid "BrD " and resid 27   and name HN  ))
  (( segid "BrD " and resid 27   and name HB1 ))
    2 500     1 600     1 600 peak  1821 weight  0.11000E+01 volume  0 78563E+03 ppm1     8 170 ppm2     4 611
ASSI { 1831}
  (( segid "BrD " and resid 27   and name HN  ))
  (( segid "BrD " and resid 26   and name HN  ))
    2 600     1.700     1 700 peak  1831 weight  0 11000E+01 volume  0 56681E+03 ppm1     8 169 ppm2     9 179
ASSI { 1851}
  (( segid "BrD " and resid 19   and name HN  ))
  (( segid "BrD " and resid 15   and name HA  ))
    3 100     2 400     2 400 peak  1851 weight  0.11000E+01 volume  0 20055E+03 ppm1     9 187 ppm2     4 645
ASSI { 1861}
  (( segid "BrD " and resid 19   and name HN  ))
  (( segid "BrD " and resid 19   and name HA  ))
    2 800     2 000     2 000 peak  1861 weight  0 11000E+01 volume  0 37223E+03 ppm1     9 189 ppm2     4 285
ASSI { 1881}
  (( segid "BrD " and resid 20   and name HN  ))
  (( segid "BrD " and resid 19   and name HN  ))
    2 800     2.000     2 000 peak  1881 weight  0 11000E+01 volume  0 39357E+03 ppm1     8.146 ppm2     9 170
ASSI { 1901}
  (( segid "BrD " and resid 83   and name HN  ))
  (( segid "BrD " and resid 83   and name HA  ))
    2 800     2.000     2.000 peak  1901 weight  0 11000E+01 volume  0 35792E+03 ppm1     9 658 ppm2     4 447
ASSI { 1911}
  (( segid "BrD " and resid 83   and name HN  ))
  (( segid "BrD " and resid 83   and name HB  ))
    2.700     1 800     1 800 peak  1911 weight  0.11000E+01 volume  0 45140E+03 ppm1     9 659 ppm2     4 817
ASSI { 1921}
  (( segid "BrD " and resid 83   and name HN  ))
  (  segid "BrD " and resid 83   and name HG2%)
    3 000     2.200     2 200 peak  1921 weight  0 11000E+01 volume  0.28097E+03 ppm1     9 659 ppm2     1 910
ASSI { 1931}
  (( segid "BrD " and resid 84   and name HN  ))
  (( segid "BrD " and resid 84   and name HA  ))
    2.800     2 000     2 000 peak  1931 weight  0 11000E+01 volume  0 37490E+03 ppm1     9.464 ppm2     4 901
ASSI { 1941}
  (( segid "BrD " and resid 84   and name HN  ))
  (( segid "BrD " and resid 84   and name HB1 ))
    2 800     2 000     2.000 peak  1941 weight  0 11000E+01 volume  0 42690E+03 ppm1     9 463 ppm2     3 592
ASSI { 1951}
  (( segid "BrD " and resid 84   and name HN  ))
  (( segid "BrD " and resid 84   and name HB2 ))
    3 000     2.200     2 200 peak  1951 weight  0 11000E+01 volume  0 26963E+03 ppm1     9 463 ppm2     3 268
ASSI { 1971}
  (( segid "BrD " and resid 83   and name HN  ))
  (( segid "BrD " and resid 84   and name HN  ))
    2 600     1 700     1 700 peak  1971 weight  0 11000E+01 volume  0 61276E+03 ppm1     9 658 ppm2     9.450
ASSI { 1981}
  (( segid "BrD " and resid 85   and name HN  ))
  (( segid "BrD " and resid 85   and name HA  ))
    2 900     2 100     2.100 peak  1981 weight  0.11000E+01 volume  0.32851E+03 ppm1     7 516 ppm2     5 014
ASSI { 1991}
  (( segid "BrD " and resid 85   and name HN  ))
  (( segid "BrD " and resid 85   and name HB1 ))
    2 800     2 000     2 000 peak  1991 weight  0 11000E+01 volume  0 39507E+03 ppm1     7 516 ppm2     3 919
ASSI { 2011}
  (( segid "BrD " and resid 84   and name HN  ))
  (( segid "BrD " and resid 85   and name HN  ))
    2 800     2.000     2.000 peak  2011 weight  0 11000E+01 volume  0 37475E+03 ppm1     9 464 ppm2     7 497
ASSI { 2021}
  (( segid "BrD " and resid 86   and name HN  ))
  (( segid "BrD " and resid 85   and name HB1 ))
    3 200     2 600     2 300 peak  2021 weight  0 11000E+01 volume  0.17051E+03 ppm1     8 423 ppm2     3 911
ASSI { 2031}
  (( segid "BrD " and resid 86   and name HN  ))
  (( segid "BrD " and resid 86   and name HA  ))
    2 800     2.000     2 000 peak  2031 weight  0 11000E+01 volume  0 42952E+03 ppm1     8.423 ppm2     4 809
ASSI { 2051}
  (( segid "BrD " and resid 85   and name HN  ))
  (( segid "BrD " and resid 86   and name HN  ))
    2 800     2 000     2.000 peak  2051 weight  0 11000E+01 volume  0 39765E+03 ppm1     7 516 ppm2     8 406
ASSI { 2061}
  (( segid "BrD " and resid 87   and name HN  ))
  (( segid "BrD " and resid 86   and name HB1 ))
    3 400     2 900     2 100 peak  2061 weight  0.11000E+01 volume  0.11283E+03 ppm1     8 570 ppm2     2 350
ASSI { 2071}
  (( segid "BrD " and resid 87   and name HN  ))
  (( segid "BrD " and resid 87   and name HA  ))
    2 600     1 700     1 700 peak  2071 weight  0 11000E+01 volume  0 62404E+03 ppm1     8 572 ppm2     4 889
ASSI { 2081}
  (( segid "BrD " and resid 87   and name HN  ))
  (( segid "BrD " and resid 87   and name HG1 ))
    3.000     2 200     2.200 peak  2081 weight  0.11000E+01 volume  0 28244E+03 ppm1     8 572 ppm2     3 014
ASSI { 2091}
  (( segid "BrD " and resid 87   and name HN  ))
  (( segid "BrD " and resid 87   and name HG2 ))
    3 000     2 200     2 200 peak  2091 weight  0 11000E+01 volume  0 28579E+03 ppm1     8 570 ppm2     2 810
ASSI { 2101}
  (( segid "BrD " and resid 87   and name HN  ))
  (( segid "BrD " and resid 87   and name HB2 ))
    2 700     1.800     1 800 peak  2101 weight  0 11000E+01 volume  0.46735E+03 ppm1     8 571 ppm2     2.607
ASSI { 2111}
  (( segid "BrD " and resid 88   and name HN  ))
  (  segid "BrD " and resid 88   and name HD% )
    3.300     2 700     2 200 peak  2111 weight  0 11000E+01 volume  0 15320E+03 ppm1     8 355 ppm2     7 595
ASSI { 2121}
  (( segid "BrD " and resid 88   and name HN  ))
  (( segid "BrD " and resid 88   and name HA  ))
    3 100     2 400     2 400 peak  2121 weight  0 11000E+01 volume  0.22276E+03 ppm1     8 356 ppm2     4 976
ASSI { 2131}
  (( segid "BrD " and resid 88   and name HN  ))
  (( segid "BrD " and resid 88   and name HB1 ))
    2 500     1 600     1.600 peak  2131 weight  0 11000E+01 volume  0.72297E+03 ppm1     8 354 ppm2     3 536
ASSI { 2151}
  (( segid "BrD " and resid 89   and name HN  ))
  (( segid "BrD " and resid 89   and name HA  ))
    3.000     2 200     2 200 peak  2151 weight  0 11000E+01 volume  0 26347E+03 ppm1     8 858 ppm2     5 631
ASSI { 2161}
  (( segid "BrD " and resid 89   and name HN  ))
  (( segid "BrD " and resid 89   and name HB1 ))
    3.000     2.200     2 200 peak  2161 weight  0 11000E+01 volume  0 26996E+03 ppm1     8.858 ppm2     3 671
ASSI { 2171}
  (( segid "BrD " and resid 89   and name HN  ))
  (( segid "BrD " and resid 89   and name HB2 ))
    2 400     1 400     1 400 peak  2171 weight  0 11000E+01 volume  0 10141E+04 ppm1     8 858 ppm2     3 508
ASSI { 2191}
  (( segid "BrD " and resid 88   and name HN  ))
  (( segid "BrD " and resid 89   and name HN  ))
    2.600     1 700     1 700 peak  2191 weight  0 11000E+01 volume  0.62488E+03 ppm1     8 355 ppm2     8 848
ASSI { 2201}
  (( segid "BrD " and resid 46   and name HN  ))
  (( segid "BrD " and resid 47   and name HN  ))
    2 800     2.000     2.000 peak  2201 weight  0.11000E+01 volume  0 38079E+03 ppm1     8 562 ppm2     8 836
ASSI { 2211}
  (( segid "BrD " and resid 46   and name HN  ))
  (( segid "BrD " and resid 46   and name HA  ))
    2 700     1.800     1 800 peak  2211 weight  0 11000E+01 volume  0.49246E+03 ppm1     8 562 ppm2     4 125
ASSI { 2221}
  (( segid "BrD " and resid 46   and name HN  ))
  (( segid "BrD " and resid 46   and name HB1 ))
    2 500     1 600     1.600 peak  2221 weight  0 11000E+01 volume  0 82312E+03 ppm1     8 561 ppm2     3 293
ASSI { 2231}
  (( segid "BrD " and resid 46   and name HN  ))
  (( segid "BrD " and resid 46   and name HB2 ))
    2.500     1.600     1 600 peak  2231 weight  0 11000E+01 volume  0 72605E+03 ppm1     8 562 ppm2     3 095
ASSI { 2241}
  (( segid "BrD " and resid 47   and name HN  ))
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  ( segid "BrD " and resid 47   and name HB% )
   3.700     3.400     1.800 peak  2241 weight  0.11000E+01 volume  0.71965E+02 ppm1     8 832 ppm2      7 253
ASSI { 2251}
  (( segid "BrD " and resid 47   and name HN  ))
  (( segid "BrD " and resid 47   and name HA  ))
   2 900     2 100     2 100 peak  2251 weight  0.11000E+01 volume  0 34426E+03 ppm1     8.831 ppm2      4 708
ASSI { 2261}
  (( segid "BrD " and resid 47   and name HN  ))
  (( segid "BrD " and resid 47   and name HB1 ))
   2 800     2 000     2 000 peak  2261 weight  0 11000E+01 volume  0 37083E+03 ppm1     8 833 ppm2      3 807
ASSI { 2271}
  (( segid "BrD " and resid 47   and name HN  ))
  (( segid "BrD " and resid 47   and name HB2 ))
   2 900     2.100     2 100 peak  2271 weight  0 11000E+01 volume  0 34763E+03 ppm1     8 832 ppm2      3 391
ASSI { 2281}
  (( segid "BrD " and resid 48   and name HN  ))
  (( segid "BrD " and resid 48   and name HA  ))
   2 800     2 000     2 000 peak  2281 weight  0 11000E+01 volume  0 37621E+03 ppm1     8 307 ppm2      4 815
ASSI { 2291}
  (( segid "BrD " and resid 48   and name HN  ))
  (( segid "BrD " and resid 48   and name HG2 ))
   3 300     2 700     2 200 peak  2291 weight  0 11000E+01 volume  0 14081E+03 ppm1     8 308 ppm2      2 857
ASSI { 2301}
  (( segid "BrD " and resid 48   and name HN  ))
  (( segid "BrD " and resid 48   and name HB1 ))
   2 400     1 400     1 400 peak  2301 weight  0 11000E+01 volume  0 11018E+04 ppm1     8 308 ppm2      2 698
ASSI { 2321}
  (( segid "BrD " and resid 47   and name HN  ))
  (( segid "BrD " and resid 48   and name HN  ))
   2 700     1 800     1 800 peak  2321 weight  0 11000E+01 volume  0 47004E+03 ppm1     8.832 ppm2      8 310
ASSI { 2341}
  (( segid "BrD " and resid 49   and name HN  ))
  (( segid "BrD " and resid 49   and name HA  ))
   2 600     1 700     1 700 peak  2341 weight  0.11000E+01 volume  0 63035E+03 ppm1     7 762 ppm2      4 690
ASSI { 2351}
  (( segid "BrD " and resid 49   and name HN  ))
  (( segid "BrD " and resid 49   and name HB  ))
   3 100     2 400     2 400 peak  2351 weight  0 11000E+01 volume  0 22961E+03 ppm1     7 762 ppm2      2 611
ASSI { 2361}
  (( segid "BrD " and resid 49   and name HN  ))
  (  segid "BrD " and resid 49   and name HG2%)
   3 300     2 700     2 200 peak  2361 weight  0.11000E+01 volume  0 15115E+03 ppm1     7 762 ppm2      1 586
ASSI { 2381}
  (( segid "BrD " and resid 48   and name HN  ))
  (( segid "BrD " and resid 49   and name HN  ))
   2 400     1 400     1 400 peak  2381 weight  0 11000E+01 volume  0 95252E+03 ppm1     8 308 ppm2      7 742
ASSI { 2391}
  (( segid "BrD " and resid 50   and name HN  ))
  (( segid "BrD " and resid 51   and name HN  ))
   2 600     1 700     1 700 peak  2391 weight  0 11000E+01 volume  0 55801E+03 ppm1     8 559 ppm2      8 318
ASSI { 2401}
  (( segid "BrD " and resid 50   and name HN  ))
  (( segid "BrD " and resid 50   and name HA  ))
   2 700     1 800     1 800 peak  2401 weight  0 11000E+01 volume  0 45800E+03 ppm1     8 564 ppm2      4.525
ASSI { 2421}
  (( segid "BrD " and resid 49   and name HN  ))
  (( segid "BrD " and resid 50   and name HN  ))
   2 400     1 400     1 400 peak  2421 weight  0.11000E+01 volume  0 91502E+03 ppm1     7.762 ppm2      8 554
ASSI { 2431}
  (( segid "BrD " and resid 115  and name HN  ))
  (( segid "BrD " and resid 114  and name HA2 ))
   3 100     2 400     2 400 peak  2431 weight  0 11000E+01 volume  0 20145E+03 ppm1     8 355 ppm2      4 542
ASSI { 2441}
  (( segid "BrD " and resid 115  and name HN  ))
  (( segid "BrD " and resid 115  and name HA  ))
   2 800     2 000     2 000 peak  2441 weight  0 11000E+01 volume  0.38387E+03 ppm1     8 355 ppm2      4 822
ASSI { 2451}
  (( segid "BrD " and resid 116  and name HN  ))
  (( segid "BrD " and resid 115  and name HB1 ))
   2 700     1 800     1 800 peak  2451 weight  0 11000E+01 volume  0 51528E+03 ppm1     8 086 ppm2      2 169
ASSI { 2461}
  (( segid "BrD " and resid 116  and name HN  ))
  (( segid "BrD " and resid 116  and name HA  ))
   2 500     1 600     1.600 peak  2461 weight  0 11000E+01 volume  0 81456E+03 ppm1     8 087 ppm2      4 828
ASSI { 2471}
  (( segid "BrD " and resid 116  and name HN  ))
  (( segid "BrD " and resid 116  and name HB  ))
   2 600     1 700     1 700 peak  2471 weight  0 11000E+01 volume  0 58085E+03 ppm1     8 086 ppm2      2 419
ASSI { 2481}
  (( segid "BrD " and resid 117  and name HN  ))
  (( segid "BrD " and resid 117  and name HA  ))
   3 300     2 700     2 200 peak  2481 weight  0.11000E+01 volume  0 15334E+03 ppm1     8 880 ppm2      5 171
ASSI { 2491}
  (( segid "BrD " and resid 117  and name HN  ))
  (( segid "BrD " and resid 117  and name HB1 ))
   3 300     2 700     2 200 peak  2491 weight  0 11000E+01 volume  0 14660E+03 ppm1     8 879 ppm2      3 300
ASSI { 2501}
  (( segid "BrD " and resid 117  and name HN  ))
  (( segid "BrD " and resid 117  and name HB2 ))
   2 800     2 000     2.000 peak  2501 weight  0 11000E+01 volume  0 41931E+03 ppm1     8 879 ppm2      3 147
ASSI { 2511}
  (( segid "BrD " and resid 51   and name HN  ))
  (( segid "BrD " and resid 51   and name HA  ))
   2 300     1 300     1 300 peak  2511 weight  0 11000E+01 volume  0 13843E+04 ppm1     8.377 ppm2      4 475
ASSI { 2521}
  (( segid "BrD " and resid 51   and name HN  ))
  (( segid "BrD " and resid 51   and name HG1 ))
   2 900     2 100     2 100 peak  2521 weight  0.11000E+01 volume  0 29957E+03 ppm1     8 375 ppm2      1 933
ASSI { 2531}
  (( segid "BrD " and resid 17   and name HN  ))
  (( segid "BrD " and resid 17   and name HB  ))
   3 000     2 200     2 200 peak  2531 weight  0 11000E+01 volume  0 26023E+03 ppm1     8 679 ppm2      4 860
ASSI { 2541}
  (( segid "BrD " and resid 17   and name HN  ))
  (( segid "BrD " and resid 17   and name HA  ))
   2 400     1 400     1 400 peak  2541 weight  0 11000E+01 volume  0 10062E+04 ppm1     8 678 ppm2      4 571
ASSI { 2551}
  (( segid "BrD " and resid 17   and name HN  ))
  (  segid "BrD " and resid 17   and name HG2%)
   3 100     2 400     2 400 peak  2551 weight  0 11000E+01 volume  0 20185E+03 ppm1     8 670 ppm2      1 745
ASSI { 2561}
  (( segid "BrD " and resid 101  and name HN  ))
  (( segid "BrD " and resid 100  and name HB2 ))
   2.800     2 000     2 000 peak  2561 weight  0 11000E+01 volume  0 38883E+03 ppm1     8 513 ppm2      3 441
ASSI { 2571}
  (( segid "BrD " and resid 101  and name HN  ))
  (( segid "BrD " and resid 101  and name HA  ))
   2 800     2.000     2 000 peak  2571 weight  0 11000E+01 volume  0 37743E+03 ppm1     8 513 ppm2      4 264
ASSI { 2591}
  (( segid "BrD " and resid 100  and name HN  ))
  (( segid "BrD " and resid 101  and name HN  ))
   2.600     1 700     1 700 peak  2591 weight  0 11000E+01 volume  0 62929E+03 ppm1     8 669 ppm2      8 521
ASSI { 2601}
  (( segid "BrD " and resid 102  and name HN  ))
  (( segid "BrD " and resid 102  and name HA  ))
   2 900     2 100     2 100 peak  2601 weight  0 11000E+01 volume  0 34745E+03 ppm1     9 156 ppm2      4 280
ASSI { 2611}
  (( segid "BrD " and resid 102  and name HN  ))
  (( segid "BrD " and resid 101  and name HN  ))
   2 700     1 800     1 800 peak  2611 weight  0 11000E+01 volume  0 52631E+03 ppm1     9 156 ppm2      8 513
ASSI { 2641}
  (( segid "BrD " and resid 103  and name HN  ))
  (( segid "BrD " and resid 103  and name HA  ))
   2 800     2 000     2 000 peak  2641 weight  0 11000E+01 volume  0 41836E+03 ppm1     8 695 ppm2      3 800
ASSI { 2651}
  (( segid "BrD " and resid 103  and name HN  ))
  (( segid "BrD " and resid 103  and name HB2 ))
   2.800     2 000     2 000 peak  2651 weight  0 11000E+01 volume  0 35593E+03 ppm1     8 696 ppm2      1.928
ASSI { 2661}
  (( segid "BrD " and resid 103  and name HN  ))
  (( segid "BrD " and resid 103  and name HB1 ))
   2 500     1 600     1 600 peak  2661 weight  0 11000E+01 volume  0 72768E+03 ppm1     8 695 ppm2      2 353
ASSI { 2671}
  (( segid "BrD " and resid 103  and name HN  ))
  (( segid "BrD " and resid 103  and name HG2 ))
   3.200     2 600     2 300 peak  2671 weight  0 11000E+01 volume  0 18331E+03 ppm1     8 695 ppm2      2 529
ASSI { 2681}
  (( segid "BrD " and resid 103  and name HN  ))
  (( segid "BrD " and resid 102  and name HN  ))
   2.600     1 700     1 700 peak  2681 weight  0.11000E+01 volume  0 68597E+03 ppm1     8 694 ppm2      9 157
ASSI { 2711}
  (( segid "BrD " and resid 104  and name HN  ))
  (( segid "BrD " and resid 104  and name HA  ))
   2.600     1 700     1 700 peak  2711 weight  0 11000E+01 volume  0 66065E+03 ppm1     7 763 ppm2      4 690
ASSI { 2731}
  (( segid "BrD " and resid 104  and name HN  ))
  (( segid "BrD " and resid 103  and name HN  ))
   2 800     2 000     2 000 peak  2731 weight  0 11000E+01 volume  0.40496E+03 ppm1     7 763 ppm2      8 680
ASSI { 2751}
  (( segid "BrD " and resid 104  and name HN  ))
  (( segid "BrD " and resid 105  and name HN  ))
   2.700     1.800     1 800 peak  2751 weight  0 11000E+01 volume  0 54532E+03 ppm1     7 763 ppm2      8.475
ASSI { 2771}
  (( segid "BrD " and resid 79   and name HN  ))
  (  segid "BrD " and resid 78   and name HD1%)
   3 900     3 800     1 600 peak  2771 weight  0 11000E+01 volume  0 50980E+02 ppm1     8 685 ppm2      0 788
ASSI { 2781}
  (( segid "BrD " and resid 81   and name HN  ))
  (( segid "BrD " and resid 81   and name HA  ))
   3.300     2 700     2 200 peak  2781 weight  0 11000E+01 volume  0 15663E+03 ppm1     7 640 ppm2      3 711
ASSI { 2791}
  (( segid "BrD " and resid 81   and name HN  ))
  (( segid "BrD " and resid 81   and name HB  ))
   2 500     1 600     1 600 peak  2791 weight  0 11000E+01 volume  0 72728E+03 ppm1     7 640 ppm2      2 037
ASSI { 2801}
  (( segid "BrD " and resid 81   and name HN  ))
  (  segid "BrD " and resid 81   and name HG1%)
   2.500     1 600     1 600 peak  2801 weight  0.11000E+01 volume  0 82553E+03 ppm1     7 640 ppm2      1 071
ASSI { 2811}
  (( segid "BrD " and resid 81   and name HN  ))
  (  segid "BrD " and resid 81   and name HG2%)
   3.100     2.400     2 400 peak  2811 weight  0.11000E+01 volume  0 22921E+03 ppm1     7 640 ppm2      0 751
ASSI { 2821}
  (( segid "BrD " and resid 82   and name HN  ))
  (  segid "BrD " and resid 82   and name HD% )
   3 000     2 200     2 200 peak  2821 weight  0 11000E+01 volume  0 28368E+03 ppm1     6.981 ppm2      7.258
ASSI { 2831}
  (( segid "BrD " and resid 82   and name HN  ))
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  (( segid "BrD " and resid 82   and name HA  ))
    2.800     2.000      2.000 peak  2831 weight  0.11000E+01 volume  0.42147E+03 ppm1      6.981 ppm2      4.738
ASSI { 2841}
  (( segid "BrD " and resid 82   and name HN  ))
  (( segid "BrD " and resid 82   and name HB1 ))
    3 000     2 200      2 200 peak  2841 weight  0 11000E+01 volume  0 27134E+03 ppm1      6 981 ppm2      3 706
ASSI { 2851}
  (( segid "BrD " and resid 82   and name HN  ))
  (( segid "BrD " and resid 82   and name HB2 ))
    2 600     1 700      1 700 peak  2851 weight  0 11000E+01 volume  0 58897E+03 ppm1      6 981 ppm2      3 556
ASSI { 2871}
  (( segid "BrD " and resid 81   and name HN  ))
  (( segid "BrD " and resid 82   and name HN  ))
    2.800     2 000      2 000 peak  2871 weight  0 11000E+01 volume  0 36428E+03 ppm1      7 640 ppm2      6 966
ASSI { 2891}
  (( segid "BrD " and resid 82   and name HN  ))
  (( segid "BrD " and resid 83   and name HN  ))
    2 800     2 000      2 000 peak  2891 weight  0 11000E+01 volume  0 41793E+03 ppm1      6 981 ppm2      9 658
ASSI { 2901}
  (( segid "BrD " and resid 79   and name HN  ))
  (  segid "BrD " and resid 78   and name HD2%)
    3.900     3 800      1 600 peak  2901 weight  0 11000E+01 volume  0 52951E+02 ppm1      8 684 ppm2      0.666
ASSI { 2911}
  (( segid "BrD " and resid 80   and name HN  ))
  (( segid "BrD " and resid 80   and name HA  ))
    2.500     1 600      1 600 peak  2911 weight  0 11000E+01 volume  0 82068E+03 ppm1      8 005 ppm2      4 678
ASSI { 2921}
  (( segid "BrD " and resid 80   and name HN  ))
  (( segid "BrD " and resid 81   and name HN  ))
    2.700     1 800      1 800 peak  2921 weight  0 11000E+01 volume  0 47132E+03 ppm1      8 006 ppm2      7 632
ASSI { 2941}
  (( segid "BrD " and resid 83   and name HN  ))
  (  segid "BrD " and resid 82   and name HD% )
    3 400     2 900      2 100 peak  2941 weight  0 11000E+01 volume  0 12712E+03 ppm1      9 658 ppm2      7 248
ASSI { 2951}
  (( segid "BrD " and resid 79   and name HN  ))
  (( segid "BrD " and resid 79   and name HA  ))
    2.600     1 700      1 700 peak  2951 weight  0 11000E+01 volume  0 57656E+03 ppm1      8.681 ppm2      4 406
ASSI { 2961}
  (( segid "BrD " and resid 79   and name HN  ))
  (( segid "BrD " and resid 79   and name HG1 ))
    2 900     2 100      2 100 peak  2961 weight  0 11000E+01 volume  0 30890E+03 ppm1      8 681 ppm2      3 055
ASSI { 2971}
  (( segid "BrD " and resid 79   and name HN  ))
  (( segid "BrD " and resid 79   and name HB2 ))
    2 500     1 600      1 600 peak  2971 weight  0 11000E+01 volume  0 78107E+03 ppm1      8 679 ppm2      2 684
ASSI { 2981}
  (( segid "BrD " and resid 80   and name HN  ))
  (( segid "BrD " and resid 79   and name HN  ))
    2 700     1 800      1 800 peak  2981 weight  0 11000E+01 volume  0 45960E+03 ppm1      8 006 ppm2      8 676
ASSI { 3001}
  (( segid "BrD " and resid 74   and name HN  ))
  (( segid "BrD " and resid 72   and name HA  ))
    3 500     3.100      2 000 peak  3001 weight  0.11000E+01 volume  0 98034E+02 ppm1      7.536 ppm2      4 666
ASSI { 3011}
  (( segid "BrD " and resid 73   and name HN  ))
  (( segid "BrD " and resid 73   and name HA  ))
    2.600     1 700      1 700 peak  3011 weight  0 11000E+01 volume  0 57896E+03 ppm1      8 045 ppm2      4 811
ASSI { 3021}
  (( segid "BrD " and resid 73   and name HN  ))
  (( segid "BrD " and resid 74   and name HN  ))
    2 800     2 000      2 000 peak  3021 weight  0 11000E+01 volume  0 42186E+03 ppm1      8 049 ppm2      7 542
ASSI { 3041}
  (( segid "BrD " and resid 64   and name HN  ))
  (( segid "BrD " and resid 63   and name HA  ))
    3.100     2 400      2 400 peak  3041 weight  0.11000E+01 volume  0 20596E+03 ppm1      8 584 ppm2      5 298
ASSI { 3051}
  (( segid "BrD " and resid 64   and name HN  ))
  (( segid "BrD " and resid 64   and name HA  ))
    2 600     1 700      1 700 peak  3051 weight  0 11000E+01 volume  0 63768E+03 ppm1      8 584 ppm2      4 940
ASSI { 3061}
  (( segid "BrD " and resid 63   and name HN  ))
  (( segid "BrD " and resid 63   and name HA  ))
    2 900     2.100      2 100 peak  3061 weight  0.11000E+01 volume  0.33289E+03 ppm1      9 473 ppm2      5 302
ASSI { 3071}
  (( segid "BrD " and resid 63   and name HN  ))
  (( segid "BrD " and resid 64   and name HN  ))
    2 600     1 700      1 700 peak  3071 weight  0 11000E+01 volume  0 68875E+03 ppm1      9 478 ppm2      8 565
ASSI { 3091}
  (( segid "BrD " and resid 38   and name HN  ))
  (( segid "BrD " and resid 38   and name HA  ))
    3.100     2 400      2 400 peak  3091 weight  0 11000E+01 volume  0 21794E+03 ppm1      8 732 ppm2      4 166
ASSI { 3101}
  (( segid "BrD " and resid 38   and name HN  ))
  (( segid "BrD " and resid 38   and name HB  ))
    2 500     1 600      1 600 peak  3101 weight  0 11000E+01 volume  0 76036E+03 ppm1      8 731 ppm2      1 767
ASSI { 3111}
  (( segid "BrD " and resid 38   and name HN  ))
  (  segid "BrD " and resid 38   and name HG1%)
    2 400     1 400      1 400 peak  3111 weight  0 11000E+01 volume  0 94284E+03 ppm1      8 733 ppm2      1 071
ASSI { 3121}
  (( segid "BrD " and resid 38   and name HN  ))
  (  segid "BrD " and resid 38   and name HG2%)
    4 000     4 000      1 500 peak  3121 weight  0 11000E+01 volume  0 47989E+02 ppm1      8 732 ppm2      0 784
ASSI { 3131}
  (( segid "BrD " and resid 39   and name HN  ))
  (( segid "BrD " and resid 39   and name HA  ))
    3 600     3 200      1 900 peak  3131 weight  0 11000E+01 volume  0 90084E+02 ppm1      9 653 ppm2      4 977
ASSI { 3141}
  (( segid "BrD " and resid 58   and name HN  ))
  (( segid "BrD " and resid 58   and name HA  ))
    2 900     2.100      2 100 peak  3141 weight  0 11000E+01 volume  0 34424E+03 ppm1     10 051 ppm2      4 451
ASSI { 3151}
  (( segid "BrD " and resid 58   and name HN  ))
  (( segid "BrD " and resid 58   and name HB  ))
    2 900     2.100      2 100 peak  3151 weight  0 11000E+01 volume  0 30448E+03 ppm1     10 052 ppm2      4 686
ASSI { 3161}
  (( segid "BrD " and resid 58   and name HN  ))
  (  segid "BrD " and resid 58   and name HG2%)
    3 700     3 400      1 800 peak  3161 weight  0 11000E+01 volume  0.68430E+02 ppm1     10 051 ppm2      1 674
ASSI { 3171}
  (( segid "BrD " and resid 57   and name HN  ))
  (( segid "BrD " and resid 57   and name HA  ))
    2 700     1 800      1 800 peak  3171 weight  0 11000E+01 volume  0 45739E+03 ppm1      9 359 ppm2      4 809
ASSI { 3191}
  (( segid "BrD " and resid 58   and name HN  ))
  (( segid "BrD " and resid 57   and name HN  ))
    2 600     1.700      1 700 peak  3191 weight  0 11000E+01 volume  0 55403E+03 ppm1     10 051 ppm2      9 351
ASSI { 3201}
  (( segid "BrD " and resid 56   and name HN  ))
  (( segid "BrD " and resid 56   and name HA  ))
    3 100     2 400      2 400 peak  3201 weight  0 11000E+01 volume  0 22011E+03 ppm1      9 678 ppm2      4.622
ASSI { 3221}
  (( segid "BrD " and resid 57   and name HN  ))
  (( segid "BrD " and resid 56   and name HN  ))
    3 100     2 400      2 400 peak  3221 weight  0.11000E+01 volume  0 21874E+03 ppm1      9 359 ppm2      9 662
ASSI { 3231}
  (( segid "BrD " and resid 79   and name HN  ))
  (( segid "BrD " and resid 78   and name HB2 ))
    3 200     2.600      2 300 peak  3231 weight  0 11000E+01 volume  0 19421E+03 ppm1      8 680 ppm2      1.049
ASSI { 3241}
  (( segid "BrD " and resid 55   and name HN  ))
  (( segid "BrD " and resid 55   and name HA  ))
    2 600     1 700      1 700 peak  3241 weight  0 11000E+01 volume  0 57256E+03 ppm1      7 973 ppm2      5 343
ASSI { 3251}
  (( segid "BrD " and resid 55   and name HN  ))
  (( segid "BrD " and resid 55   and name HB1 ))
    3.200     2 600      2 300 peak  3251 weight  0 11000E+01 volume  0 19260E+03 ppm1      7.975 ppm2      2 971
ASSI { 3271}
  (( segid "BrD " and resid 16   and name HN  ))
  (( segid "BrD " and resid 16   and name HA  ))
    2 500     1 600      1 600 peak  3271 weight  0 11000E+01 volume  0 81267E+03 ppm1      8 792 ppm2      4 514
ASSI { 3281}
  (( segid "BrD " and resid 15   and name HN  ))
  (( segid "BrD " and resid 11   and name HA  ))
    3 600     3 200      1 900 peak  3281 weight  0 11000E+01 volume  0.88513E+02 ppm1      8 599 ppm2      4 936
ASSI { 3291}
  (( segid "BrD " and resid 15   and name HN  ))
  (( segid "BrD " and resid 15   and name HA  ))
    3.000     2.200      2 200 peak  3291 weight  0 11000E+01 volume  0 23859E+03 ppm1      8 599 ppm2      4 615
ASSI { 3301}
  (( segid "BrD " and resid 15   and name HN  ))
  (( segid "BrD " and resid 15   and name HB1 ))
    2 600     1 700      1 700 peak  3301 weight  0 11000E+01 volume  0 66455E+03 ppm1      8 598 ppm2      3 809
ASSI { 3311}
  (( segid "BrD " and resid 15   and name HN  ))
  (( segid "BrD " and resid 15   and name HB2 ))
    2 500     1.600      1 600 peak  3311 weight  0.11000E+01 volume  0 74771E+03 ppm1      8 598 ppm2      3 634
ASSI { 3331}
  (( segid "BrD " and resid 16   and name HN  ))
  (( segid "BrD " and resid 15   and name HN  ))
    2 500     1 600      1 600 peak  3331 weight  0 11000E+01 volume  0 87721E+03 ppm1      8 793 ppm2      8 628
ASSI { 3341}
  (( segid "BrD " and resid 13   and name HN  ))
  (( segid "BrD " and resid 13   and name HA  ))
    3.200     2 600      2 300 peak  3341 weight  0 11000E+01 volume  0.16876E+03 ppm1      8 801 ppm2      4 773
ASSI { 3351}
  (( segid "BrD " and resid 14   and name HN  ))
  (( segid "BrD " and resid 14   and name HA  ))
    3 300     2 700      2 200 peak  3351 weight  0.11000E+01 volume  0 15715E+03 ppm1      8.811 ppm2      4.651
ASSI { 3381}
  (( segid "BrD " and resid 13   and name HN  ))
  (( segid "BrD " and resid 13   and name HB1 ))
    2 300     1 300      1.300 peak  3381 weight  0 11000E+01 volume  0 12106E+04 ppm1      8 807 ppm2      2 758
ASSI { 3391}
  (( segid "BrD " and resid 14   and name HN  ))
  (( segid "BrD " and resid 11   and name HA  ))
    3 300     2.700      2.200 peak  3391 weight  0 11000E+01 volume  0 15172E+03 ppm1      8 809 ppm2      4 939
ASSI { 3411}
  (( segid "BrD " and resid 34   and name HN  ))
  (( segid "BrD " and resid 34   and name HA  ))
    2.800     2.000      2.000 peak  3411 weight  0 11000E+01 volume  0 39310E+03 ppm1      8.176 ppm2      5 542
ASSI { 3421}
  (( segid "BrD " and resid 34   and name HN  ))
  (( segid "BrD " and resid 34   and name HB1 ))
    3 600     3 200      1 900 peak  3421 weight  0.11000E+01 volume  0 86588E+02 ppm1      8 182 ppm2      4 098
ASSI { 3431}
  (( segid "BrD " and resid 34   and name HN  ))
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  (( segid "BrD " and resid 34   and name HB2 ))
     2.700     1.800     1.800 peak  3431 weight  0.11000E+01 volume  0 51957E+03 ppm1      8.182 ppm2      3.143
ASSI { 3441}
  (( segid "BrD " and resid 35   and name HN  ))
  (( segid "BrD " and resid 34   and name HB2 ))
     3 300     2 700     2 200 peak  3441 weight  0 11000E+01 volume  0 14464E+03 ppm1      7 735 ppm2      3 139
ASSI { 3451}
  (( segid "BrD " and resid 35   and name HN  ))
  (( segid "BrD " and resid 35   and name HA  ))
     2.800     2 000     2.000 peak  3451 weight  0 11000E+01 volume  0 42792E+03 ppm1      7 734 ppm2      4 899
ASSI { 3461}
  (( segid "BrD " and resid 35   and name HN  ))
  (( segid "BrD " and resid 35   and name HG1 ))
     2 700     1 800     1 800 peak  3461 weight  0 11000E+01 volume  0 54517E+03 ppm1      7 734 ppm2      3 436
ASSI { 3471}
  (( segid "BrD " and resid 35   and name HN  ))
  (( segid "BrD " and resid 35   and name HB2 ))
     3 300     2 700     2.200 peak  3471 weight  0 11000E+01 volume  0 15293E+03 ppm1      7 733 ppm2      2 781
ASSI { 3491}
  (( segid "BrD " and resid 34   and name HN  ))
  (( segid "BrD " and resid 35   and name HN  ))
     2 200     1 200     1 200 peak  3491 weight  0.11000E+01 volume  0 15285E+04 ppm1      8 176 ppm2      7 714
ASSI { 3501}
  (( segid "BrD " and resid 36   and name HN  ))
  (( segid "BrD " and resid 36   and name HA  ))
     2 600     1 700     1 700 peak  3501 weight  0 11000E+01 volume  0 56896E+03 ppm1      8 310 ppm2      5.456
ASSI { 3511}
  (( segid "BrD " and resid 36   and name HN  ))
  (( segid "BrD " and resid 36   and name HG1 ))
     3 700     3 400     1.800 peak  3511 weight  0 11000E+01 volume  0 72744E+02 ppm1      8.308 ppm2      2.771
ASSI { 3521}
  (( segid "BrD " and resid 36   and name HN  ))
  (( segid "BrD " and resid 36   and name HB2 ))
     2 600     1 700     1 700 peak  3521 weight  0 11000E+01 volume  0 65455E+03 ppm1      8 311 ppm2      2 337
ASSI { 3541}
  (( segid "BrD " and resid 35   and name HN  ))
  (( segid "BrD " and resid 36   and name HN  ))
     2 700     1 800     1 800 peak  3541 weight  0 11000E+01 volume  0 54251E+03 ppm1      7 734 ppm2      8 316
ASSI { 3561}
  (( segid "BrD " and resid 12   and name HN  ))
  (( segid "BrD " and resid 12   and name HA  ))
     2 100     1 100     1 100 peak  3561 weight  0 11000E+01 volume  0 19935E+04 ppm1      9 021 ppm2      5 292
ASSI { 3571}
  (( segid "BrD " and resid 12   and name HN  ))
  (( segid "BrD " and resid 12   and name HB1 ))
     2 700     1 800     1.800 peak  3571 weight  0 11000E+01 volume  0 46239E+03 ppm1      9 020 ppm2      3.428
ASSI { 3581}
  (( segid "BrD " and resid 10   and name HN  ))
  (( segid "BrD " and resid 10   and name HA  ))
     3 500     3 100     2 000 peak  3581 weight  0 11000E+01 volume  0 10021E+03 ppm1      8 885 ppm2      5 481
ASSI { 3591}
  (( segid "BrD " and resid 10   and name HN  ))
  (( segid "BrD " and resid 10   and name HB1 ))
     3 000     2 200     2 200 peak  3591 weight  0 11000E+01 volume  0 27522E+03 ppm1      8.885 ppm2      3.361
ASSI { 3611}
  (( segid "BrD " and resid 9    and name HN  ))
  (( segid "BrD " and resid 9    and name HB1 ))
     2 900     2 100     2 100 peak  3611 weight  0.11000E+01 volume  0 31864E+03 ppm1      9 054 ppm2      2 444
ASSI { 3621}
  (( segid "BrD " and resid 9    and name HN  ))
  (( segid "BrD " and resid 10   and name HN  ))
     3 500     3 100     2.000 peak  3621 weight  0 11000E+01 volume  0 11024E+03 ppm1      9 054 ppm2      8 880
ASSI { 3641}
  (( segid "BrD " and resid 62   and name HN  ))
  (( segid "BrD " and resid 62   and name HD1 ))
     3.400     2 900     2 100 peak  3641 weight  0 11000E+01 volume  0 12186E+03 ppm1      8 998 ppm2      3 185
ASSI { 3651}
  (( segid "BrD " and resid 62   and name HN  ))
  (( segid "BrD " and resid 61   and name HG2 ))
     3 000     2 200     2 200 peak  3651 weight  0 11000E+01 volume  0 24395E+03 ppm1      8.999 ppm2      2 783
ASSI { 3661}
  (( segid "BrD " and resid 62   and name HN  ))
  (( segid "BrD " and resid 62   and name HG1 ))
     2 600     1 700     1 700 peak  3661 weight  0 11000E+01 volume  0 63487E+03 ppm1      8 997 ppm2      2 329
ASSI { 3681}
  (( segid "BrD " and resid 7    and name HN  ))
  (( segid "BrD " and resid 7    and name HA  ))
     3 100     2 400     2 400 peak  3681 weight  0 11000E+01 volume  0 21276E+03 ppm1      8 924 ppm2      5 147
ASSI { 3691}
  (( segid "BrD " and resid 7    and name HN  ))
  (( segid "BrD " and resid 7    and name HG1 ))
     3 400     2 900     2.100 peak  3691 weight  0.11000E+01 volume  0 12947E+03 ppm1      8.923 ppm2      2 878
ASSI { 3701}
  (( segid "BrD " and resid 7    and name HN  ))
  (( segid "BrD " and resid 7    and name HB1 ))
     3 100     2 400     2 400 peak  3701 weight  0.11000E+01 volume  0.20103E+03 ppm1      8 923 ppm2      2 631
ASSI { 3711}
  (( segid "BrD " and resid 7    and name HN  ))
  (( segid "BrD " and resid 7    and name HB2 ))
     2.700     1 800     1 800 peak  3711 weight  0.11000E+01 volume  0 54229E+03 ppm1      8 924 ppm2      2.500
ASSI { 3721}
  (( segid "BrD " and resid 79   and name HN  ))
  (( segid "BrD " and resid 78   and name HG  ))
     2.800     2 000     2 000 peak  3721 weight  0.11000E+01 volume  0.38659E+03 ppm1      8 681 ppm2      1.314
ASSI { 3731}
  (( segid "BrD " and resid 78   and name HN  ))
  (( segid "BrD " and resid 78   and name HA  ))
     2 500     1 600     1 600 peak  3731 weight  0 11000E+01 volume  0 73125E+03 ppm1      7 996 ppm2      4 004
ASSI { 3741}
  (( segid "BrD " and resid 118  and name HN  ))
  (( segid "BrD " and resid 118  and name HA  ))
     2.900     2 100     2 100 peak  3741 weight  0 11000E+01 volume  0 30830E+03 ppm1      8 381 ppm2      4 689
ASSI { 3761}
  (( segid "BrD " and resid 54   and name HN  ))
  (( segid "BrD " and resid 54   and name HA  ))
     2 900     2 100     2 100 peak  3761 weight  0 11000E+01 volume  0 30432E+03 ppm1      9 036 ppm2      5 546
ASSI { 3771}
  (( segid "BrD " and resid 54   and name HN  ))
  (( segid "BrD " and resid 54   and name HB1 ))
     3 400     2 900     2 100 peak  3771 weight  0 11000E+01 volume  0 12506E+03 ppm1      9 036 ppm2      2.596
ASSI { 3781}
  (( segid "BrD " and resid 54   and name HN  ))
  (( segid "BrD " and resid 54   and name HB2 ))
     3.600     3 200     1 900 peak  3781 weight  0 11000E+01 volume  0 92666E+02 ppm1      9 037 ppm2      1 960
ASSI { 3791}
  (( segid "BrD " and resid 62   and name HN  ))
  (( segid "BrD " and resid 59   and name HA  ))
     3 200     2 600     2 300 peak  3791 weight  0 11000E+01 volume  0 18605E+03 ppm1      8 998 ppm2      4 900
ASSI { 3801}
  (( segid "BrD " and resid 62   and name HN  ))
  (( segid "BrD " and resid 62   and name HA  ))
     2.800     2 000     2 000 peak  3801 weight  0.11000E+01 volume  0 36964E+03 ppm1      8 998 ppm2      4 467
ASSI { 3811}
  (( segid "BrD " and resid 72   and name HN  ))
  (( segid "BrD " and resid 72   and name HA  ))
     3.000     2 200     2 200 peak  3811 weight  0 11000E+01 volume  0.24473E+03 ppm1      8 858 ppm2      4.648
ASSI { 3821}
  (( segid "BrD " and resid 72   and name HN  ))
  (( segid "BrD " and resid 73   and name HN  ))
     3.700     3 400     1 800 peak  3821 weight  0 11000E+01 volume  0 74895E+02 ppm1      8 858 ppm2      8 033
ASSI { 3851}
  (( segid "BrD " and resid 61   and name HN  ))
  (( segid "BrD " and resid 61   and name HA  ))
     2 500     1 600     1.600 peak  3851 weight  0 11000E+01 volume  0 82145E+03 ppm1      8 748 ppm2      4.652
ASSI { 3861}
  (( segid "BrD " and resid 65   and name HN  ))
  (( segid "BrD " and resid 62   and name HA  ))
     3 100     2 400     2 400 peak  3861 weight  0 11000E+01 volume  0 22227E+03 ppm1      8 568 ppm2      4 476
ASSI { 3871}
  (( segid "BrD " and resid 60   and name HN  ))
  (( segid "BrD " and resid 60   and name HA  ))
     2 400     1 400     1 400 peak  3871 weight  0 11000E+01 volume  0 10791E+04 ppm1      8 569 ppm2      4 808
ASSI { 3881}
  (( segid "BrD " and resid 60   and name HN  ))
  (( segid "BrD " and resid 60   and name HB2 ))
     2 400     1 400     1 400 peak  3881 weight  0 11000E+01 volume  0.10099E+04 ppm1      8 569 ppm2      4 647
ASSI { 3891}
  (( segid "BrD " and resid 60   and name HN  ))
  (( segid "BrD " and resid 60   and name HB1 ))
     2.600     1 700     1 700 peak  3891 weight  0 11000E+01 volume  0 65212E+03 ppm1      8 568 ppm2      4.975
ASSI { 3901}
  (( segid "BrD " and resid 59   and name HN  ))
  (( segid "BrD " and resid 59   and name HA  ))
     3.200     2.600     2 300 peak  3901 weight  0.11000E+01 volume  0 18755E+03 ppm1      8 497 ppm2      4.893
ASSI { 3921}
  (( segid "BrD " and resid 7    and name HN  ))
  (( segid "BrD " and resid 6    and name HA  ))
     2 600     1 700     1 700 peak  3921 weight  0.11000E+01 volume  0 63166E+03 ppm1      8 924 ppm2      4 968
ASSI { 3931}
  (( segid "BrD " and resid 10   and name HN  ))
  (( segid "BrD " and resid 9    and name HA  ))
     2 600     1 700     1.700 peak  3931 weight  0 11000E+01 volume  0 55346E+03 ppm1      8.884 ppm2      4 938
ASSI { 3941}
  (( segid "BrD " and resid 13   and name HN  ))
  (( segid "BrD " and resid 12   and name HA  ))
     3 200     2.600     2 300 peak  3941 weight  0 11000E+01 volume  0.18205E+03 ppm1      8 809 ppm2      5 299
ASSI { 3951}
  (( segid "BrD " and resid 16   and name HN  ))
  (( segid "BrD " and resid 15   and name HB1 ))
     3 300     2 700     2 200 peak  3951 weight  0 11000E+01 volume  0 13722E+03 ppm1      8 793 ppm2      3 818
ASSI { 3961}
  (( segid "BrD " and resid 16   and name HN  ))
  (( segid "BrD " and resid 15   and name HB2 ))
     2 500     1 600     1 600 peak  3961 weight  0 11000E+01 volume  0 74092E+03 ppm1      8 793 ppm2      3 631
ASSI { 3971}
  (( segid "BrD " and resid 17   and name HN  ))
  (( segid "BrD " and resid 16   and name HA  ))
     2.500     1 600     1.600 peak  3971 weight  0.11000E+01 volume  0 82685E+03 ppm1      8 669 ppm2      4 516
ASSI { 3991}
  (( segid "BrD " and resid 18   and name HN  ))
  (( segid "BrD " and resid 18   and name HA  ))
     3.000     2 200     2 200 peak  3991 weight  0 11000E+01 volume  0 24581E+03 ppm1      9.072 ppm2      3.878
ASSI { 4001}
  (( segid "BrD " and resid 18   and name HN  ))
  (( segid "BrD " and resid 17   and name HB  ))
     2 800     2.000     2 000 peak  4001 weight  0 11000E+01 volume  0 36663E+03 ppm1      9 072 ppm2      4 854
ASSI { 4011}
  (( segid "BrD " and resid 18   and name HN  ))
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  (( segid "BrD " and resid 17   and name HA  ))
     3.200     2.600     2.300 peak  4011 weight  0.11000E+01 volume  0.18724E+03 ppm1     9.072 ppm2     4.531
ASSI { 4021}
  (( segid "BrD " and resid 18   and name HN  ))
  (  segid "BrD " and resid 17   and name HG2%)
     3 100     2 400     2 400 peak  4021 weight  0 11000E+01 volume  0 23212E+03 ppm1     9 073 ppm2     1 749
ASSI { 4041}
  (( segid "BrD " and resid 17   and name HN  ))
  (( segid "BrD " and resid 18   and name HN  ))
     2.600     1 700     1 700 peak  4041 weight  0.11000E+01 volume  0 57514E+03 ppm1     8 669 ppm2     9 062
ASSI { 4051}
  (( segid "BrD " and resid 19   and name HN  ))
  (( segid "BrD " and resid 18   and name HA  ))
     3.500     3 100     2 000 peak  4051 weight  0 11000E+01 volume  0.95460E+02 ppm1     9 187 ppm2     3 878
ASSI { 4061}
  (( segid "BrD " and resid 20   and name HN  ))
  (( segid "BrD " and resid 19   and name HA  ))
     3 200     2 600     2 300 peak  4061 weight  0 11000E+01 volume  0 17148E+03 ppm1     8 146 ppm2     4 288
ASSI { 4071}
  (( segid "BrD " and resid 21   and name HN  ))
  (( segid "BrD " and resid 20   and name HA  ))
     3.400     2 900     2 100 peak  4071 weight  0 11000E+01 volume  0 11425E+03 ppm1     8 545 ppm2     4 889
ASSI { 4081}
  (( segid "BrD " and resid 22   and name HN  ))
  (( segid "BrD " and resid 21   and name HA  ))
     3.300     2.700     2 200 peak  4081 weight  0 11000E+01 volume  0 15238E+03 ppm1     9 457 ppm2     4.361
ASSI { 4091}
  (( segid "BrD " and resid 23   and name HN  ))
  (( segid "BrD " and resid 22   and name HA  ))
     3 600     3.200     1 900 peak  4091 weight  0.11000E+01 volume  0 91130E+02 ppm1     9 118 ppm2     4 734
ASSI { 4101}
  (( segid "BrD " and resid 24   and name HN  ))
  (( segid "BrD " and resid 23   and name HA  ))
     3 500     3 100     2 000 peak  4101 weight  0 11000E+01 volume  0 11008E+03 ppm1     8 661 ppm2     4 640
ASSI { 4111}
  (( segid "BrD " and resid 25   and name HN  ))
  (( segid "BrD " and resid 24   and name HA  ))
     3 300     2 700     2 200 peak  4111 weight  0 11000E+01 volume  0 14843E+03 ppm1     9 133 ppm2     4 753
ASSI { 4121}
  (( segid "BrD " and resid 25   and name HN  ))
  (( segid "BrD " and resid 24   and name HG2 ))
     2 500     1 600     1 600 peak  4121 weight  0 11000E+01 volume  0 87462E+03 ppm1     9 131 ppm2     3 059
ASSI { 4141}
  (( segid "BrD " and resid 27   and name HN  ))
  (( segid "BrD " and resid 26   and name HA  ))
     3 200     2 600     2 300 peak  4141 weight  0 11000E+01 volume  0.18491E+03 ppm1     8 171 ppm2     4 493
ASSI { 4151}
  (( segid "BrD " and resid 28   and name HN  ))
  (( segid "BrD " and resid 27   and name HA  ))
     3 300     2 700     2 200 peak  4151 weight  0 11000E+01 volume  0 14739E+03 ppm1     8 166 ppm2     5.055
ASSI { 4161}
  (( segid "BrD " and resid 29   and name HN  ))
  (( segid "BrD " and resid 28   and name HA  ))
     2 400     1.400     1 400 peak  4161 weight  0 11000E+01 volume  0 91502E+03 ppm1     9 151 ppm2     4 574
ASSI { 4171}
  (( segid "BrD " and resid 29   and name HN  ))
  (( segid "BrD " and resid 28   and name HB1 ))
     3 400     2 900     2 100 peak  4171 weight  0 11000E+01 volume  0 11906E+03 ppm1     9 151 ppm2     3 597
ASSI { 4181}
  (( segid "BrD " and resid 29   and name HN  ))
  (( segid "BrD " and resid 28   and name HB2 ))
     3 800     3.600     1 700 peak  4181 weight  0 11000E+01 volume  0.65813E+02 ppm1     9 152 ppm2     3 406
ASSI { 4191}
  (( segid "BrD " and resid 30   and name HN  ))
  (( segid "BrD " and resid 29   and name HA  ))
     3.600     3 200     1 900 peak  4191 weight  0.11000E+01 volume  0 88464E+02 ppm1    12 275 ppm2     4 819
ASSI { 4201}
  (( segid "BrD " and resid 30   and name HN  ))
  (( segid "BrD " and resid 29   and name HB1 ))
     3.400     2.900     2 100 peak  4201 weight  0 11000E+01 volume  0 11541E+03 ppm1    12 275 ppm2     2 718
ASSI { 4211}
  (( segid "BrD " and resid 30   and name HN  ))
  (( segid "BrD " and resid 29   and name HG1 ))
     3.600     3.200     1 900 peak  4211 weight  0 11000E+01 volume  0 88536E+02 ppm1    12 275 ppm2     3.024
ASSI { 4221}
  (( segid "BrD " and resid 31   and name HN  ))
  (( segid "BrD " and resid 30   and name HA  ))
     3.600     3 200     1 900 peak  4221 weight  0.11000E+01 volume  0 86531E+02 ppm1     8.481 ppm2     5 449
ASSI { 4231}
  (( segid "BrD " and resid 31   and name HN  ))
  (( segid "BrD " and resid 30   and name HB1 ))
     3 000     2 200     2.200 peak  4231 weight  0 11000E+01 volume  0 23699E+03 ppm1     8 480 ppm2     4 941
ASSI { 4241}
  (( segid "BrD " and resid 31   and name HN  ))
  (( segid "BrD " and resid 30   and name HB2 ))
     3 500     3.100     2 000 peak  4241 weight  0 11000E+01 volume  0.10932E+03 ppm1     8 480 ppm2     4 533
ASSI { 4251}
  (( segid "BrD " and resid 68   and name HN  ))
  (( segid "BrD " and resid 67   and name HB1 ))
     2 700     1 800     1.800 peak  4251 weight  0 11000E+01 volume  0 47519E+03 ppm1     8 627 ppm2     3 555
ASSI { 4261}
  (( segid "BrD " and resid 32   and name HN  ))
  (  segid "BrD " and resid 31   and name HB% )
     2 900     2 100     2 100 peak  4261 weight  0 11000E+01 volume  0 35188E+03 ppm1     7 739 ppm2     2 295
ASSI { 4271}
  (( segid "BrD " and resid 32   and name HN  ))
  (( segid "BrD " and resid 31   and name HN  ))
     2 300     1 300     1 300 peak  4271 weight  0 11000E+01 volume  0 11812E+04 ppm1     7 739 ppm2     8 475
ASSI { 4291}
  (( segid "BrD " and resid 35   and name HN  ))
  (( segid "BrD " and resid 34   and name HA  ))
     3 200     2 600     2 300 peak  4291 weight  0 11000E+01 volume  0.17960E+03 ppm1     7 734 ppm2     5.537
ASSI { 4301}
  (( segid "BrD " and resid 36   and name HN  ))
  (( segid "BrD " and resid 37   and name HD1 ))
     3 500     3.100     2 000 peak  4301 weight  0 11000E+01 volume  0 97101E+02 ppm1     8 309 ppm2     4 277
ASSI { 4311}
  (( segid "BrD " and resid 36   and name HN  ))
  (( segid "BrD " and resid 35   and name HA  ))
     3 300     2 700     2 200 peak  4311 weight  0 11000E+01 volume  0 16106E+03 ppm1     8 308 ppm2     4 893
ASSI { 4321}
  (( segid "BrD " and resid 36   and name HN  ))
  (( segid "BrD " and resid 35   and name HG1 ))
     3 700     3 400     1 800 peak  4321 weight  0 11000E+01 volume  0 78555E+02 ppm1     8 307 ppm2     3 458
ASSI { 4331}
  (( segid "BrD " and resid 39   and name HN  ))
  (( segid "BrD " and resid 38   and name HA  ))
     2 200     1 200     1 200 peak  4331 weight  0.11000E+01 volume  0 15683E+04 ppm1     9 652 ppm2     4 160
ASSI { 4341}
  (( segid "BrD " and resid 39   and name HN  ))
  (( segid "BrD " and resid 38   and name HB  ))
     3 400     2.900     2 100 peak  4341 weight  0 11000E+01 volume  0 11939E+03 ppm1     9 652 ppm2     1 752
ASSI { 4351}
  (( segid "BrD " and resid 39   and name HN  ))
  (  segid "BrD " and resid 38   and name HG1%)
     3 600     3 200     1 900 peak  4351 weight  0 11000E+01 volume  0 93234E+02 ppm1     9 652 ppm2     1.071
ASSI { 4361}
  (( segid "BrD " and resid 39   and name HN  ))
  (  segid "BrD " and resid 38   and name HG2%)
     3.100     2 400     2 400 peak  4361 weight  0 11000E+01 volume  0 20061E+03 ppm1     9 652 ppm2     0 776
ASSI { 4381}
  (( segid "BrD " and resid 43   and name HN  ))
  (( segid "BrD " and resid 42   and name HA  ))
     2 900     2 100     2 100 peak  4381 weight  0 11000E+01 volume  0 31481E+03 ppm1     8.001 ppm2     5 055
ASSI { 4391}
  (( segid "BrD " and resid 43   and name HN  ))
  (( segid "BrD " and resid 42   and name HB2 ))
     2 800     2 000     2 000 peak  4391 weight  0 11000E+01 volume  0 36989E+03 ppm1     8 001 ppm2     2 607
ASSI { 4401}
  (( segid "BrD " and resid 43   and name HN  ))
  (( segid "BrD " and resid 42   and name HB1 ))
     2 900     2 100     2 100 peak  4401 weight  0 11000E+01 volume  0 32280E+03 ppm1     8 001 ppm2     2 781
ASSI { 4411}
  (( segid "BrD " and resid 36   and name HN  ))
  (( segid "BrD " and resid 36   and name HB1 ))
     2 800     2 000     2 000 peak  4411 weight  0 11000E+01 volume  0 42122E+03 ppm1     8 308 ppm2     2 698
ASSI { 4421}
  (( segid "BrD " and resid 47   and name HN  ))
  (( segid "BrD " and resid 46   and name HA  ))
     3 300     2 700     2 200 peak  4421 weight  0 11000E+01 volume  0 14320E+03 ppm1     8 832 ppm2     4 139
ASSI { 4431}
  (( segid "BrD " and resid 47   and name HN  ))
  (( segid "BrD " and resid 46   and name HB1 ))
     3 500     3 100     2 000 peak  4431 weight  0 11000E+01 volume  0 11013E+03 ppm1     8 832 ppm2     3.296
ASSI { 4441}
  (( segid "BrD " and resid 47   and name HN  ))
  (( segid "BrD " and resid 46   and name HB2 ))
     3.100     2.400     2 400 peak  4441 weight  0.11000E+01 volume  0.20297E+03 ppm1     8.833 ppm2     3.094
ASSI { 4451}
  (( segid "BrD " and resid 48   and name HN  ))
  (( segid "BrD " and resid 47   and name HA  ))
     3 200     2 600     2 300 peak  4451 weight  0 11000E+01 volume  0.16849E+03 ppm1     8 307 ppm2     4 708
ASSI { 4461}
  (( segid "BrD " and resid 49   and name HN  ))
  (( segid "BrD " and resid 48   and name HA  ))
     3.000     2 200     2 200 peak  4461 weight  0.11000E+01 volume  0 24376E+03 ppm1     7 762 ppm2     4 816
ASSI { 4471}
  (( segid "BrD " and resid 49   and name HN  ))
  (( segid "BrD " and resid 48   and name HG2 ))
     4.000     4 000     1.500 peak  4471 weight  0 11000E+01 volume  0 45441E+02 ppm1     7 762 ppm2     2.872
ASSI { 4481}
  (( segid "BrD " and resid 49   and name HN  ))
  (( segid "BrD " and resid 48   and name HB1 ))
     3 200     2 600     2 300 peak  4481 weight  0.11000E+01 volume  0 17937E+03 ppm1     7 762 ppm2     2 693
ASSI { 4491}
  (( segid "BrD " and resid 50   and name HN  ))
  (( segid "BrD " and resid 49   and name HA  ))
     2 600     1.700     1 700 peak  4491 weight  0 11000E+01 volume  0 60014E+03 ppm1     8 564 ppm2     4.693
ASSI { 4501}
  (( segid "BrD " and resid 50   and name HN  ))
  (( segid "BrD " and resid 49   and name HB  ))
     2.900     2 100     2 100 peak  4501 weight  0.11000E+01 volume  0 31627E+03 ppm1     8 564 ppm2     2.622
ASSI { 4511}
  (( segid "BrD " and resid 50   and name HN  ))
  (  segid "BrD " and resid 49   and name HG2%)
     3.700     3.400     1.800 peak  4511 weight  0 11000E+01 volume  0 77577E+02 ppm1     8 564 ppm2     1 598
ASSI { 4521}
  (( segid "BrD " and resid 55   and name HN  ))
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  (( segid "BrD " and resid 54   and name HA  ))
     2.300     1.300     1.300 peak  4521 weight  0.11000E+01 volume  0.11556E+04 ppm1      7.974 ppm2      5.542
ASSI ( 4531)
  (( segid "BrD " and resid 55   and name HN  ))
  (( segid "BrD " and resid 54   and name HB1 ))
     3 700     3 400     1 800 peak  4531 weight  0 11000E+01 volume  0 71474E+02 ppm1      7 975 ppm2      2 572
ASSI ( 4541)
  (( segid "BrD " and resid 55   and name HN  ))
  (( segid "BrD " and resid 54   and name HB2 ))
     3 100     2 400     2 400 peak  4541 weight  0 11000E+01 volume  0 20373E+03 ppm1      7.975 ppm2      1 956
ASSI ( 4551)
  (( segid "BrD " and resid 56   and name HN  ))
  (( segid "BrD " and resid 55   and name HA  ))
     2 800     2 000     2.000 peak  4551 weight  0.11000E+01 volume  0 38353E+03 ppm1      9 676 ppm2      5 352
ASSI ( 4561)
  (( segid "BrD " and resid 56   and name HN  ))
  (( segid "BrD " and resid 55   and name HB1 ))
     2 400     1 400     1 400 peak  4561 weight  0 11000E+01 volume  0 92127E+03 ppm1      9 679 ppm2      2 978
ASSI ( 4571)
  (( segid "BrD " and resid 57   and name HN  ))
  (( segid "BrD " and resid 56   and name HA  ))
     3 200     2 600     2 300 peak  4571 weight  0 11000E+01 volume  0 16116E+03 ppm1      9 359 ppm2      4 648
ASSI ( 4581)
  (( segid "BrD " and resid 58   and name HN  ))
  (( segid "BrD " and resid 57   and name HA  ))
     3 400     2 900     2 100 peak  4581 weight  0 11000E+01 volume  0 12185E+03 ppm1     10 050 ppm2      4 805
ASSI ( 4591)
  (( segid "BrD " and resid 59   and name HN  ))
  (( segid "BrD " and resid 58   and name HA  ))
     3 400     2 900     2 100 peak  4591 weight  0 11000E+01 volume  0 13191E+03 ppm1      8 498 ppm2      4 449
ASSI ( 4601)
  (( segid "BrD " and resid 59   and name HN  ))
  (( segid "BrD " and resid 58   and name HB  ))
     3 200     2.600     2 300 peak  4601 weight  0 11000E+01 volume  0 18613E+03 ppm1      8 498 ppm2      4 697
ASSI ( 4611)
  (( segid "BrD " and resid 59   and name HN  ))
  (  segid "BrD " and resid 58   and name HG2%)
     3 100     2 400     2 400 peak  4611 weight  0 11000E+01 volume  0 21128E+03 ppm1      8.496 ppm2      1 665
ASSI ( 4631)
  (( segid "BrD " and resid 58   and name HN  ))
  (( segid "BrD " and resid 59   and name HN  ))
     3 200     2 600     2 300 peak  4631 weight  0.11000E+01 volume  0 17034E+03 ppm1     10 051 ppm2      8 489
ASSI ( 4641)
  (( segid "BrD " and resid 61   and name HN  ))
  (( segid "BrD " and resid 61   and name HG1 ))
     2 400     1 400     1 400 peak  4641 weight  0 11000E+01 volume  0 89496E+03 ppm1      8 743 ppm2      2 974
ASSI ( 4651)
  (( segid "BrD " and resid 61   and name HN  ))
  (( segid "BrD " and resid 61   and name HB2 ))
     2 500     1 600     1 600 peak  4651 weight  0 11000E+01 volume  0 72876E+03 ppm1      8 743 ppm2      2 670
ASSI ( 4661)
  (( segid "BrD " and resid 61   and name HN  ))
  (( segid "BrD " and resid 60   and name HA  ))
     3 300     2 700     2 200 peak  4661 weight  0 11000E+01 volume  0 14220E+03 ppm1      8 749 ppm2      4 816
ASSI ( 4691)
  (( segid "BrD " and resid 60   and name HN  ))
  (( segid "BrD " and resid 61   and name HN  ))
     2 400     1 400     1 400 peak  4691 weight  0 11000E+01 volume  0 96369E+03 ppm1      8 566 ppm2      8 734
ASSI ( 4701)
  (( segid "BrD " and resid 62   and name HN  ))
  (( segid "BrD " and resid 61   and name HA  ))
     3 200     2 600     2 300 peak  4701 weight  0 11000E+01 volume  0 17192E+03 ppm1      8 997 ppm2      4 656
ASSI ( 4711)
  (( segid "BrD " and resid 63   and name HN  ))
  (( segid "BrD " and resid 62   and name HN  ))
     2 800     2 000     2 000 peak  4711 weight  0 11000E+01 volume  0 35764E+03 ppm1      9 477 ppm2      8 998
ASSI ( 4731)
  (( segid "BrD " and resid 63   and name HN  ))
  (( segid "BrD " and resid 62   and name HA  ))
     3 600     3 200     1.900 peak  4731 weight  0.11000E+01 volume  0 90728E+02 ppm1      9 472 ppm2      4.481
ASSI ( 4741)
  (( segid "BrD " and resid 65   and name HD21))
  (( segid "BrD " and resid 65   and name HB1 ))
     3 500     3 100     2.000 peak  4741 weight  0 11000E+01 volume  0 10454E+03 ppm1      8 206 ppm2      3 637
ASSI ( 4751)
  (( segid "BrD " and resid 65   and name HD22))
  (( segid "BrD " and resid 65   and name HB1 ))
     3 500     3 100     2 000 peak  4751 weight  0 11000E+01 volume  0 97769E+02 ppm1      7.576 ppm2      3.637
ASSI ( 4761)
  (( segid "BrD " and resid 65   and name HD21))
  (( segid "BrD " and resid 65   and name HB2 ))
     3.200     2 600     2 300 peak  4761 weight  0.11000E+01 volume  0.17538E+03 ppm1      8 205 ppm2      3 393
ASSI ( 4771)
  (( segid "BrD " and resid 65   and name HD22))
  (( segid "BrD " and resid 65   and name HB2 ))
     3.400     2 900     2 100 peak  4771 weight  0 11000E+01 volume  0 13182E+03 ppm1      7 576 ppm2      3 393
ASSI ( 4781)
  (( segid "BrD " and resid 24   and name HE21))
  (( segid "BrD " and resid 24   and name HG1 ))
     3 400     2 900     2.100 peak  4781 weight  0 11000E+01 volume  0.11561E+03 ppm1      7 634 ppm2      3.459
ASSI ( 4791)
  (( segid "BrD " and resid 24   and name HE22))
  (( segid "BrD " and resid 24   and name HG1 ))
     3 600     3 200     1.900 peak  4791 weight  0 11000E+01 volume  0 90206E+02 ppm1      7 523 ppm2      3 474
ASSI ( 4801)
  (( segid "BrD " and resid 66   and name HN  ))
  (( segid "BrD " and resid 65   and name HA  ))
     2 700     1 800     1 800 peak  4801 weight  0 11000E+01 volume  0 48168E+03 ppm1      8.762 ppm2      5 378
ASSI ( 4811)
  (( segid "BrD " and resid 66   and name HN  ))
  (( segid "BrD " and resid 65   and name HB1 ))
     3 400     2 900     2 100 peak  4811 weight  0 11000E+01 volume  0 11537E+03 ppm1      8 759 ppm2      3 608
ASSI ( 4821)
  (( segid "BrD " and resid 66   and name HN  ))
  (( segid "BrD " and resid 65   and name HB2 ))
     3 300     2 700     2 200 peak  4821 weight  0 11000E+01 volume  0 13853E+03 ppm1      8 763 ppm2      3 381
ASSI ( 4831)
  (( segid "BrD " and resid 67   and name HN  ))
  (( segid "BrD " and resid 66   and name HA  ))
     2 800     2.000     2 000 peak  4831 weight  0.11000E+01 volume  0 41855E+03 ppm1      8 832 ppm2      5 009
ASSI ( 4841)
  (( segid "BrD " and resid 68   and name HN  ))
  (( segid "BrD " and resid 67   and name HA  ))
     3 400     2 900     2 100 peak  4841 weight  0 11000E+01 volume  0 12732E+03 ppm1      8 627 ppm2      4 671
ASSI ( 4851)
  (( segid "BrD " and resid 68   and name HN  ))
  (( segid "BrD " and resid 67   and name HB2 ))
     3.300     2 700     2 200 peak  4851 weight  0.11000E+01 volume  0 15213E+03 ppm1      8 626 ppm2      2.662
ASSI ( 4861)
  (( segid "BrD " and resid 69   and name HN  ))
  (( segid "BrD " and resid 68   and name HA  ))
     2 400     1 400     1 400 peak  4861 weight  0 11000E+01 volume  0 95815E+03 ppm1      8 305 ppm2      5 141
ASSI ( 4871)
  (( segid "BrD " and resid 69   and name HN  ))
  (( segid "BrD " and resid 68   and name HB1 ))
     4 500     4.500     1 000 peak  4871 weight  0 11000E+01 volume  0 22391E+02 ppm1      8 306 ppm2      3 669
ASSI ( 4881)
  (( segid "BrD " and resid 69   and name HN  ))
  (( segid "BrD " and resid 68   and name HB2 ))
     3 300     2 700     2 200 peak  4881 weight  0.11000E+01 volume  0 15981E+03 ppm1      8 306 ppm2      3 514
ASSI ( 4891)
  (( segid "BrD " and resid 70   and name HN  ))
  (( segid "BrD " and resid 69,  and name HA  ))
     3 000     2 200     2 200 peak  4891 weight  0 11000E+01 volume  0 24443E+03 ppm1      8.039 ppm2      4 690
ASSI ( 4901)
  (( segid "BrD " and resid 70   and name HN  ))
  (( segid "BrD " and resid 69   and name HB  ))
     3.400     2 900     2 100 peak  4901 weight  0.11000E+01 volume  0 12954E+03 ppm1      8 040 ppm2      2 928
ASSI ( 4911)
  (( segid "BrD " and resid 70   and name HN  ))
  (  segid "BrD " and resid 69   and name HG1%)
     3 800     3 600     1 700 peak  4911 weight  0 11000E+01 volume  0 61869E+02 ppm1      8 041 ppm2      1 551
ASSI ( 4921)
  (( segid "BrD " and resid 70   and name HN  ))
  (  segid "BrD " and resid 69   and name HG2%)
     2 700     1 800     1 800 peak  4921 weight  0 11000E+01 volume  0 48346E+03 ppm1      8 040 ppm2      1 430
ASSI ( 4931)
  (( segid "BrD " and resid 73   and name HN  ))
  (( segid "BrD " and resid 72   and name HA  ))
     2 900     2 100     2 100 peak  4931 weight  0 11000E+01 volume  0 30696E+03 ppm1      8.045 ppm2      4 654
ASSI ( 4941)
  (( segid "BrD " and resid 74   and name HN  ))
  (( segid "BrD " and resid 73   and name HA  ))
     3.500     3 100     2 000 peak  4941 weight  0.11000E+01 volume  0.10430E+03 ppm1      7.536 ppm2      4 812
ASSI ( 4951)
  (( segid "BrD " and resid 75   and name HN  ))
  (( segid "BrD " and resid 74   and name HA  ))
     3 500     3 100     2 000 peak  4951 weight  0.11000E+01 volume  0 10099E+03 ppm1      9 106 ppm2      4 361
ASSI ( 4961)
  (( segid "BrD " and resid 76   and name HN  ))
  (( segid "BrD " and resid 75   and name HA  ))
     3.400     2 900     2 100 peak  4961 weight  0 11000E+01 volume  0 11734E+03 ppm1      8.611 ppm2      4 525
ASSI ( 4971)
  (( segid "BrD " and resid 76   and name HN  ))
  (( segid "BrD " and resid 75   and name HG1 ))
     3 000     2 200     2 200 peak  4971 weight  0 11000E+01 volume  0 28328E+03 ppm1      8 611 ppm2      3 549
ASSI ( 4981)
  (( segid "BrD " and resid 76   and name HN  ))
  (( segid "BrD " and resid 75   and name HG2 ))
     3.200     2.600     2 300 peak  4981 weight  0 11000E+01 volume  0 18815E+03 ppm1      8 610 ppm2      3 218
ASSI ( 4991)
  (( segid "BrD " and resid 76   and name HN  ))
  (( segid "BrD " and resid 75   and name HB2 ))
     2.600     1 700     1 700 peak  4991 weight  0 11000E+01 volume  0 61964E+03 ppm1      8.611 ppm2      2 815
ASSI ( 5001)
  (( segid "BrD " and resid 76   and name HN  ))
  (( segid "BrD " and resid 75   and name HB1 ))
     2.600     1.700     1.700 peak  5001 weight  0.11000E+01 volume  0 59739E+03 ppm1      8 611 ppm2      2 925
ASSI ( 5011)
  (( segid "BrD " and resid 77   and name HN  ))
  (( segid "BrD " and resid 76   and name HA  ))
     3.000     2.200     2 200 peak  5011 weight  0 11000E+01 volume  0 25554E+03 ppm1      7.996 ppm2      4 695
ASSI ( 5021)
  (( segid "BrD " and resid 77   and name HN  ))
  (  segid "BrD " and resid 76   and name HB% )
     2 500     1 600     1 600 peak  5021 weight  0.11000E+01 volume  0 86259E+03 ppm1      7 996 ppm2      2 092
ASSI ( 5031)
  (( segid "BrD " and resid 79   and name HN  ))
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  (( segid "BrD " and resid 78   and name HA  ))
     3.300     2.700     2 200 peak  5031 weight  0 11000E+01 volume  0 14659E+03 ppm1      8 681 ppm2      3 995
ASSI { 5041}
  (( segid "BrD " and resid 78   and name HN  ))
  (( segid "BrD " and resid 79   and name HN  ))
     2 400     1 400     1 400 peak  5041 weight  0 11000E+01 volume  0 10403E+04 ppm1      7 996 ppm2      8 687
ASSI { 5061}
  (( segid "BrD " and resid 80   and name HN  ))
  (( segid "BrD " and resid 80   and name HD1 ))
     5 300     5 300     0 200 peak  5061 weight  0 11000E+01 volume  0 85899E+01 ppm1      8 006 ppm2      3 997
ASSI { 5071}
  (( segid "BrD " and resid 80   and name HN  ))
  (( segid "BrD " and resid 79   and name HA  ))
     3 300     2 700     2.200 peak  5071 weight  0 11000E+01 volume  0 15955E+03 ppm1      8 006 ppm2      4 404
ASSI { 5091}
  (( segid "BrD " and resid 80   and name HN  ))
  (( segid "BrD " and resid 79   and name HB2 ))
     3 200     2 600     2 300 peak  5091 weight  0 11000E+01 volume  0 16421E+03 ppm1      8 006 ppm2      2 704
ASSI { 5101}
  (( segid "BrD " and resid 81   and name HN  ))
  (( segid "BrD " and resid 80   and name HA  ))
     3 700     3.400     1 800 peak  5101 weight  0.11000E+01 volume  0 77456E+02 ppm1      7 639 ppm2      4 685
ASSI { 5111}
  (( segid "BrD " and resid 82   and name HN  ))
  (( segid "BrD " and resid 81   and name HB  ))
     2 500     1 600     1 600 peak  5111 weight  0 11000E+01 volume  0 81882E+03 ppm1      6 981 ppm2      2 042
ASSI { 5121}
  (( segid "BrD " and resid 82   and name HN  ))
  (  segid "BrD " and resid 81   and name HG1%)
     3 200     2 600     2 300 peak  5121 weight  0 11000E+01 volume  0 17066E+03 ppm1      6 981 ppm2      1 086
ASSI { 5131}
  (( segid "BrD " and resid 82   and name HN  ))
  (  segid "BrD " and resid 81   and name HG2%)
     3 400     2 900     2 100 peak  5131 weight  0 11000E+01 volume  0 12101E+03 ppm1      6 981 ppm2      0 749
ASSI { 5141}
  (( segid "BrD " and resid 83   and name HN  ))
  (( segid "BrD " and resid 82   and name HA  ))
     3 400     2 900     2 100 peak  5141 weight  0 11000E+01 volume  0 11364E+03 ppm1      9 658 ppm2      4 743
ASSI { 5151}
  (( segid "BrD " and resid 83   and name HN  ))
  (( segid "BrD " and resid 82   and name HB1 ))
     3 500     3 100     2 000 peak  5151 weight  0 11000E+01 volume  0 10752E+03 ppm1      9 660 ppm2      3.697
ASSI { 5161}
  (( segid "BrD " and resid 83   and name HN  ))
  (( segid "BrD " and resid 82   and name HB2 ))
     2 800     2 000     2 000 peak  5161 weight  0 11000E+01 volume  0 41394E+03 ppm1      9 658 ppm2      3 551
ASSI { 5171}
  (( segid "BrD " and resid 84   and name HN  ))
  (( segid "BrD " and resid 83   and name HB  ))
     3 200     2 600     2 300 peak  5171 weight  0 11000E+01 volume  0 19086E+03 ppm1      9 466 ppm2      4 817
ASSI { 5181}
  (( segid "BrD " and resid 84   and name HN  ))
  (( segid "BrD " and resid 83   and name HA  ))
     3 600     3 200     1 900 peak  5181 weight  0 11000E+01 volume  0 83498E+02 ppm1      9.463 ppm2      4 449
ASSI { 5191}
  (( segid "BrD " and resid 84   and name HN  ))
  (  segid "BrD " and resid 83   and name HG2%)
     3.500     3 100     2 000 peak  5191 weight  0 11000E+01 volume  0 11050E+03 ppm1      9.463 ppm2      1 903
ASSI { 5201}
  (( segid "BrD " and resid 85   and name HN  ))
  (( segid "BrD " and resid 84   and name HA  ))
     3.700     3.400     1 800 peak  5201 weight  0 11000E+01 volume  0 79848E+02 ppm1      7 515 ppm2      4 921
ASSI { 5211}
  (( segid "BrD " and resid 85   and name HN  ))
  (( segid "BrD " and resid 84   and name HB2 ))
     3 400     2 900     2.100 peak  5211 weight  0.11000E+01 volume  0.12439E+03 ppm1      7 516 ppm2      3 268
ASSI { 5221}
  (( segid "BrD " and resid 86   and name HN  ))
  (( segid "BrD " and resid 85   and name HA  ))
     3.900     3 800     1.600 peak  5221 weight  0 11000E+01 volume  0 50221E+02 ppm1      8 423 ppm2      5 012
ASSI { 5231}
  (( segid "BrD " and resid 86   and name HN  ))
  (( segid "BrD " and resid 85   and name HB2 ))
     3.300     2 700     2 200 peak  5231 weight  0 11000E+01 volume  0 14503E+03 ppm1      8 423 ppm2      3 639
ASSI { 5241}
  (( segid "BrD " and resid 87   and name HN  ))
  (( segid "BrD " and resid 86   and name HA  ))
     3 600     3 200     1 900 peak  5241 weight  0 11000E+01 volume  0 84494E+02 ppm1      8 572 ppm2      4 815
ASSI { 5251}
  (( segid "BrD " and resid 88   and name HN  ))
  (( segid "BrD " and resid 87   and name HA  ))
     3.600     3 200     1 900 peak  5251 weight  0 11000E+01 volume  0 87457E+02 ppm1      8 357 ppm2      4 857
ASSI { 5261}
  (( segid "BrD " and resid 88   and name HN  ))
  (( segid "BrD " and resid 87   and name HB1 ))
     3.100     2 400     2 400 peak  5261 weight  0 11000E+01 volume  0 23456E+03 ppm1      8.354 ppm2      2 782
ASSI { 5271}
  (( segid "BrD " and resid 88   and name HN  ))
  (( segid "BrD " and resid 87   and name HB2 ))
     3.200     2 600     2 300 peak  5271 weight  0 11000E+01 volume  0 19424E+03 ppm1      8 354 ppm2      2 614
ASSI { 5281}
  (( segid "BrD " and resid 88   and name HN  ))
  (( segid "BrD " and resid 87   and name HN  ))
     2.600     1 700     1 700 peak  5281 weight  0 11000E+01 volume  0 67695E+03 ppm1      8 355 ppm2      8 552
ASSI { 5301}
  (( segid "BrD " and resid 89   and name HN  ))
  (( segid "BrD " and resid 88   and name HA  ))
     3.400     2 900     2 100 peak  5301 weight  0 11000E+01 volume  0 12542E+03 ppm1      8 858 ppm2      4 976
ASSI { 5311}
  (( segid "BrD " and resid 89   and name HD21))
  (( segid "BrD " and resid 89   and name HB2 ))
     3.900     3.800     1.600 peak  5311 weight  0 11000E+01 volume  0 54504E+02 ppm1      8 923 ppm2      3 516
ASSI { 5321}
  (( segid "BrD " and resid 89   and name HD22))
  (( segid "BrD " and resid 89   and name HB2 ))
     3 300     2.700     2 200 peak  5321 weight  0 11000E+01 volume  0 13631E+03 ppm1      8 416 ppm2      3.514
ASSI { 5331}
  (( segid "BrD " and resid 89   and name HD21))
  (( segid "BrD " and resid 89   and name HB1 ))
     5 100     5 100     0 400 peak  5331 weight  0 11000E+01 volume  0 10399E+02 ppm1      8 923 ppm2      3.679
ASSI { 5341}
  (( segid "BrD " and resid 89   and name HD22))
  (( segid "BrD " and resid 89   and name HB1 ))
     3 900     3 800     1 600 peak  5341 weight  0 11000E+01 volume  0 50137E+02 ppm1      8 416 ppm2      3.676
ASSI { 5351}
  (( segid "BrD " and resid 92   and name HN  ))
  (( segid "BrD " and resid 92   and name HG1 ))
     2 700     1 800     1 800 peak  5351 weight  0 11000E+01 volume  0 53011E+03 ppm1      8 876 ppm2      2 818
ASSI { 5361}
  (( segid "BrD " and resid 92   and name HN  ))
  (( segid "BrD " and resid 92   and name HB1 ))
     3 600     3 200     1 900 peak  5361 weight  0.11000E+01 volume  0 93326E+02 ppm1      8 875 ppm2      2 697
ASSI { 5371}
  (( segid "BrD " and resid 92   and name HN  ))
  (( segid "BrD " and resid 92   and name HB2 ))
     2.500     1.600     1 600 peak  5371 weight  0.11000E+01 volume  0 87608E+03 ppm1      8 875 ppm2      2 576
ASSI { 5381}
  (( segid "BrD " and resid 93   and name HN  ))
  (( segid "BrD " and resid 92   and name HG1 ))
     3.500     3 100     2 000 peak  5381 weight  0 11000E+01 volume  0 10524E+03 ppm1      8 714 ppm2      2 807
ASSI { 5391}
  (( segid "BrD " and resid 93   and name HN  ))
  (( segid "BrD " and resid 92   and name HB1 ))
     3.200     2 600     2 300 peak  5391 weight  0 11000E+01 volume  0 16925E+03 ppm1      8 714 ppm2      2 702
ASSI { 5401}
  (( segid "BrD " and resid 93   and name HN  ))
  (( segid "BrD " and resid 92   and name HB2 ))
     3 300     2 700     2 200 peak  5401 weight  0 11000E+01 volume  0 13613E+03 ppm1      8.714 ppm2      2 580
ASSI { 5411}
  (( segid "BrD " and resid 94   and name HN  ))
  (( segid "BrD " and resid 94   and name HB1 ))
     2 700     1 800     1 800 peak  5411 weight  0 11000E+01 volume  0 51785E+03 ppm1      9 677 ppm2      2.777
ASSI { 5421}
  (( segid "BrD " and resid 94   and name HN  ))
  (( segid "BrD " and resid 94   and name HG1 ))
     3 600     3 200     1 900 peak  5421 weight  0 11000E+01 volume  0.85031E+02 ppm1      9 679 ppm2      3 144
ASSI { 5431}
  (( segid "BrD " and resid 94   and name HN  ))
  (( segid "BrD " and resid 93   and name HA  ))
     3.300     2 700     2 200 peak  5431 weight  0 11000E+01 volume  0 15989E+03 ppm1      9 678 ppm2      5 042
ASSI { 5441}
  (( segid "BrD " and resid 94   and name HN  ))
  (( segid "BrD " and resid 93   and name HB2 ))
     3 000     2 200     2 200 peak  5441 weight  0 11000E+01 volume  0 25357E+03 ppm1      9.680 ppm2      4.764
ASSI { 5451}
  (( segid "BrD " and resid 95   and name HN  ))
  (( segid "BrD " and resid 94   and name HA  ))
     3 600     3 200     1 900 peak  5451 weight  0.11000E+01 volume  0 81131E+02 ppm1      8 669 ppm2      4.839
ASSI { 5461}
  (( segid "BrD " and resid 95   and name HN  ))
  (( segid "BrD " and resid 94   and name HG1 ))
     3 400     2 900     2 100 peak  5461 weight  0 11000E+01 volume  0 12127E+03 ppm1      8 669 ppm2      3 135
ASSI { 5471}
  (( segid "BrD " and resid 95   and name HN  ))
  (( segid "BrD " and resid 94   and name HB1 ))
     2 800     2.000     2 000 peak  5471 weight  0 11000E+01 volume  0 41579E+03 ppm1      8 670 ppm2      2 776
ASSI { 5481}
  (( segid "BrD " and resid 96   and name HN  ))
  (( segid "BrD " and resid 95   and name HN  ))
     2 400     1 400     1 400 peak  5481 weight  0.11000E+01 volume  0 91814E+03 ppm1      7 979 ppm2      8.679
ASSI { 5501}
  (( segid "BrD " and resid 97   and name HN  ))
  (( segid "BrD " and resid 96   and name HA  ))
     3.300     2 700     2 200 peak  5501 weight  0 11000E+01 volume  0 15786E+03 ppm1      8 677 ppm2      4 426
ASSI { 5511}
  (( segid "BrD " and resid 97   and name HN  ))
  (( segid "BrD " and resid 96   and name HB1 ))
     3.200     2.600     2 300 peak  5511 weight  0 11000E+01 volume  0 17339E+03 ppm1      8 674 ppm2      3.997
ASSI { 5521}
  (( segid "BrD " and resid 97   and name HN  ))
  (( segid "BrD " and resid 96   and name HB2 ))
     3 000     2.200     2 200 peak  5521 weight  0 11000E+01 volume  0 24048E+03 ppm1      8.674 ppm2      3 107
ASSI { 5531}
  (( segid "BrD " and resid 99   and name HN  ))
  (( segid "BrD " and resid 98   and name HA  ))
     3 200     2.600     2 300 peak  5531 weight  0 11000E+01 volume  0 16985E+03 ppm1      8 936 ppm2      4.813
ASSI { 5541}
  (( segid "BrD " and resid 99   and name HN  ))
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(( segid "BrD " and resid 98   and name HB1 ))
   3 200    2 600    2 300 peak  5541 weight  0 11000E+01 volume  0.16699E+03 ppm1     8 936 ppm2     4 003
ASSI { 5551}
  (( segid "BrD " and resid 99   and name HN  ))
  (( segid "BrD " and resid 98   and name HB2 ))
   2 900    2 100    2 100 peak  5551 weight  0 11000E+01 volume  0 29941E+03 ppm1     8.936 ppm2     3 663
ASSI { 5561}
  (( segid "BrD " and resid 100  and name HN  ))
  (( segid "BrD " and resid 99   and name HA  ))
   3 300    2 700    2 200 peak  5561 weight  0 11000E+01 volume  0 14856E+03 ppm1     8 669 ppm2     4 438
ASSI { 5571}
  (( segid "BrD " and resid 100  and name HN  ))
  (  segid "BrD " and resid 99   and name HB% )
   2.600    1 700    1 700 peak  5571 weight  0 11000E+01 volume  0.56660E+03 ppm1     8 669 ppm2     2.204
ASSI { 5581}
  (( segid "BrD " and resid 101  and name HN  ))
  (( segid "BrD " and resid 100  and name HA  ))
   3 500    3 100    2 000 peak  5581 weight  0 11000E+01 volume  0 99135E+02 ppm1     8 513 ppm2     4 940
ASSI { 5591}
  (( segid "BrD " and resid 101  and name HN  ))
  (( segid "BrD " and resid 100  and name HB1 ))
   3 200    2 600    2 300 peak  5591 weight  0 11000E+01 volume  0 18321E+03 ppm1     8.513 ppm2     3 484
ASSI { 5601}
  (( segid "BrD " and resid 102  and name HN  ))
  (( segid "BrD " and resid 101  and name HA  ))
   3 500    3 100    2.000 peak  5601 weight  0 11000E+01 volume  0 10380E+03 ppm1     9 156 ppm2     4.256
ASSI { 5611}
  (( segid "BrD " and resid 103  and name HN  ))
  (( segid "BrD " and resid 102  and name HA  ))
   3 500    3 100    2 000 peak  5611 weight  0 11000E+01 volume  0 10037E+03 ppm1     8 696 ppm2     4 277
ASSI { 5621}
  (( segid "BrD " and resid 104  and name HN  ))
  (( segid "BrD " and resid 103  and name HA  ))
   3 200    2 600    2 300 peak  5621 weight  0.11000E+01 volume  0 16539E+03 ppm1     7 763 ppm2     3.792
ASSI { 5631}
  (( segid "BrD " and resid 104  and name HN  ))
  (( segid "BrD " and resid 103  and name HB1 ))
   2 800    2 000    2.000 peak  5631 weight  0 11000E+01 volume  0 39404E+03 ppm1     7 762 ppm2     2 327
ASSI { 5641}
  (( segid "BrD " and resid 104  and name HN  ))
  (( segid "BrD " and resid 103  and name HB2 ))
   3 200    2 600    2 300 peak  5641 weight  0 11000E+01 volume  0 16250E+03 ppm1     7 763 ppm2     1 917
ASSI { 5651}
  (( segid "BrD " and resid 105  and name HN  ))
  (( segid "BrD " and resid 104  and name HA  ))
   3 200    2 600    2 300 peak  5651 weight  0 11000E+01 volume  0 16160E+03 ppm1     8 488 ppm2     4 688
ASSI { 5661}
  (( segid "BrD " and resid 106  and name HN  ))
  (( segid "BrD " and resid 105  and name HA  ))
   3.600    3 200    1.900 peak  5661 weight  0.11000E+01 volume  0 94653E+02 ppm1     9 740 ppm2     4 934
ASSI { 5671}
  (( segid "BrD " and resid 107  and name HN  ))
  (( segid "BrD " and resid 106  and name HA  ))
   3 500    3 100    2 000 peak  5671 weight  0 11000E+01 volume  0 10620E+03 ppm1     8 981 ppm2     4 568
ASSI { 5681}
  (( segid "BrD " and resid 107  and name HN  ))
  (( segid "BrD " and resid 106  and name HB1 ))
   3 000    2 200    2 200 peak  5681 weight  0 11000E+01 volume  0 25814E+03 ppm1     8 980 ppm2     3 896
ASSI { 5691}
  (( segid "BrD " and resid 108  and name HN  ))
  (( segid "BrD " and resid 107  and name HA  ))
   3 200    2 600    2 300 peak  5691 weight  0 11000E+01 volume  0 17635E+03 ppm1     8 526 ppm2     4 447
ASSI { 5701}
  (( segid "BrD " and resid 108  and name HN  ))
  (( segid "BrD " and resid 107  and name HB1 ))
   2 600    1.700    1 700 peak  5701 weight  0 11000E+01 volume  0 68256E+03 ppm1     8 526 ppm2     3 671
ASSI { 5711}
  (( segid "BrD " and resid 109  and name HN  ))
  (( segid "BrD " and resid 108  and name HA  ))
   3 700    3 400    1 800 peak  5711 weight  0 11000E+01 volume  0.77637E+02 ppm1     8 574 ppm2     4 818
ASSI { 5721}
  (( segid "BrD " and resid 110  and name HN  ))
  (( segid "BrD " and resid 109  and name HA  ))
   3 700    3 400    1.800 peak  5721 weight  0 11000E+01 volume  0 78233E+02 ppm1     8 714 ppm2     4 615
ASSI { 5731}
  (( segid "BrD " and resid 111  and name HN  ))
  (( segid "BrD " and resid 110  and name HA  ))
   3 000    2.200    2.200 peak  5731 weight  0 11000E+01 volume  0.28368E+03 ppm1     8 168 ppm2     4 428
ASSI { 5741}
  (( segid "BrD " and resid 111  and name HN  ))
  (( segid "BrD " and resid 110  and name HB  ))
   2 300    1 300    1 300 peak  5741 weight  0.11000E+01 volume  0 13983E+04 ppm1     8.170 ppm2     2 353
ASSI { 5751}
  (( segid "BrD " and resid 111  and name HN  ))
  (( segid "BrD " and resid 112  and name HN  ))
   2 800    2 000    2 000 peak  5751 weight  0 11000E+01 volume  0.38572E+03 ppm1     8 168 ppm2     8 665
ASSI { 5761}
  (( segid "BrD " and resid 113  and name HN  ))
  (( segid "BrD " and resid 112  and name HA  ))
   2.700    1 800    1 800 peak  5761 weight  0.11000E+01 volume  0 46496E+03 ppm1     8.217 ppm2     4 602
ASSI { 5771}
  (( segid "BrD " and resid 113  and name HN  ))
  (( segid "BrD " and resid 112  and name HG1 ))
   3 800    3 600    1.700 peak  5771 weight  0.11000E+01 volume  0 63604E+02 ppm1     8.216 ppm2     2.949
ASSI { 5781}
  (( segid "BrD " and resid 113  and name HN  ))
  (( segid "BrD " and resid 112  and name HG2 ))
   4 100    4 100    1.400 peak  5781 weight  0 11000E+01 volume  0 37977E+02 ppm1     8 217 ppm2     2 812
ASSI { 5791}
  (( segid "BrD " and resid 113  and name HN  ))
  (( segid "BrD " and resid 112  and name HB1 ))
   2.500    1.600    1 600 peak  5791 weight  0 11000E+01 volume  0 72974E+03 ppm1     8 217 ppm2     2.665
ASSI { 5801}
  (( segid "BrD " and resid 112  and name HN  ))
  (( segid "BrD " and resid 113  and name HN  ))
   2 500    1 600    1 600 peak  5801 weight  0 11000E+01 volume  0 81801E+03 ppm1     8 668 ppm2     8 185
ASSI { 5811}
  (( segid "BrD " and resid 114  and name HN  ))
  (( segid "BrD " and resid 113  and name HA  ))
   3.400    2 900    2.100 peak  5811 weight  0.11000E+01 volume  0 12247E+03 ppm1     8 376 ppm2     4.898
ASSI { 5821}
  (( segid "BrD " and resid 114  and name HN  ))
  (  segid "BrD " and resid 113  and name HB% )
   3 000    2.200    2.200 peak  5821 weight  0 11000E+01 volume  0 28680E+03 ppm1     8 377 ppm2     1 965
ASSI { 5831}
  (( segid "BrD " and resid 115  and name HN  ))
  (( segid "BrD " and resid 114  and name HA1 ))
   3.500    3 100    2 000 peak  5831 weight  0 11000E+01 volume  0 95188E+02 ppm1     8 355 ppm2     4 626
ASSI { 5851}
  (( segid "BrD " and resid 115  and name HN  ))
  (( segid "BrD " and resid 116  and name HN  ))
   3 700    3 400    1 800 peak  5851 weight  0 11000E+01 volume  0 76519E+02 ppm1     8 355 ppm2     8 065
ASSI { 5861}
  (( segid "BrD " and resid 117  and name HN  ))
  (( segid "BrD " and resid 116  and name HA  ))
   2.600    1 700    1 700 peak  5861 weight  0 11000E+01 volume  0 60302E+03 ppm1     8 884 ppm2     4 839
ASSI { 5871}
  (( segid "BrD " and resid 117  and name HN  ))
  (( segid "BrD " and resid 116  and name HB  ))
   3 100    2 400    2 400 peak  5871 weight  0 11000E+01 volume  0 21223E+03 ppm1     8 876 ppm2     2 417
ASSI { 5881}
  (( segid "BrD " and resid 118  and name HN  ))
  (( segid "BrD " and resid 117  and name HA  ))
   2 500    1 600    1 600 peak  5881 weight  0 11000E+01 volume  0 81728E+03 ppm1     8 381 ppm2     5 178
ASSI { 5891}
  (( segid "BrD " and resid 79   and name HE21))
  (( segid "BrD " and resid 79   and name HG1 ))
   3 900    3 800    1 600 peak  5891 weight  0 11000E+01 volume  0 58235F+02 ppm1     7 926 ppm2     3 067
ASSI { 5901}
  (( segid "BrD " and resid 79   and name HE22))
  (( segid "BrD " and resid 79   and name HG1 ))
   3.500    3 100    2 000 peak  5901 weight  0 11000E+01 volume  0 10842E+03 ppm1     7 829 ppm2     3 067
ASSI { 5911}
  (( segid "BrD " and resid 29   and name HE21))
  (( segid "BrD " and resid 29   and name HG1 ))
   4 200    4 200    1 300 peak  5911 weight  0 11000E+01 volume  0 35552E+02 ppm1     8 188 ppm2     3 028
ASSI { 5921}
  (( segid "BrD " and resid 29   and name HE22))
  (( segid "BrD " and resid 29   and name HG1 ))
   3.800    3.600    1.700 peak  5921 weight  0 11000E+01 volume  0 59289E+02 ppm1     7 477 ppm2     3 028
ASSI { 5931}
  (( segid "BrD " and resid 70   and name HN  ))
  (( segid "BrD " and resid 70   and name HB1 ))
   3 300    2 700    2 200 peak  5931 weight  0 11000E+01 volume  0 15569E+03 ppm1     8 039 ppm2     4 807
ASSI { 5941}
  (( segid "BrD " and resid 18   and name HN  ))
  (( segid "BrD " and resid 18   and name HB1 ))
   2.700    1 800    1 800 peak  5941 weight  0 11000E+01 volume  0 45519E+03 ppm1     9 072 ppm2     2 113
ASSI { 5951}
  (( segid "BrD " and resid 18   and name HN  ))
  (( segid "BrD " and resid 18   and name HG  ))
   2.600    1 700    1 700 peak  5951 weight  0 11000E+01 volume  0 60681E+03 ppm1     9 072 ppm2     2 279
ASSI { 5961}
  (( segid "BrD " and resid 18   and name HN  ))
  (  segid "BrD " and resid 18   and name HD2%)
   3 000    2.200    2 200 peak  5961 weight  0 11000E+01 volume  0 24628E+03 ppm1     9 076 ppm2     0 416
ASSI { 5971}
  (( segid "BrD " and resid 78   and name HN  ))
  (( segid "BrD " and resid 78   and name HB1 ))
   3.000    2 200    2 200 peak  5971 weight  0.11000E+01 volume  0 24153E+03 ppm1     7 996 ppm2     1 360
ASSI { 5981}
  (( segid "BrD " and resid 78   and name HN  ))
  (( segid "BrD " and resid 78   and name HB2 ))
   2 600    1 700    1 700 peak  5981 weight  0.11000E+01 volume  0 64225E+03 ppm1     7.996 ppm2     1 048
ASSI { 5991}
  (( segid "BrD " and resid 78   and name HN  ))
  (  segid "BrD " and resid 78   and name HD2%)
   3 500    3 100    2 000 peak  5991 weight  0 11000E+01 volume  0 10124E+03 ppm1     7 994 ppm2     0 667
ASSI { 6001}
  (( segid "BrD " and resid 78   and name HN  ))
  (( segid "BrD " and resid 78   and name HG  ))
   3 000    2 200    2 200 peak  6001 weight  0 11000E+01 volume  0 26923E+03 ppm1     7 996 ppm2     1 293
ASSI { 6011}
  (( segid "BrD " and resid 78   and name HN  ))
  (  segid "BrD " and resid 78   and name HD1%)
   3.500    3 100    2 000 peak  6011 weight  0 11000E+01 volume  0.10789E+03 ppm1     7 996 ppm2     0 790
ASSI { 6021}
  (( segid "BrD " and resid 115  and name HN  ))
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(( segid "BrD " and resid 115  and name HB1 ))
   3 200     2 600     2.300 peak  6021 weight  0.11000E+01 volume  0 18336E+03 ppm1     8 355 ppm2     2 167
ASSI { 6031}
 (( segid "BrD " and resid 115  and name HN  ))
 (  segid "BrD " and resid 115  and name HD1%)
   2 800     2 000     2 000 peak  6031 weight  0 11000E+01 volume  0 43402E+03 ppm1     8 354 ppm2     1 318
ASSI { 6041}
 (( segid "BrD " and resid 116  and name HN  ))
 (( segid "BrD " and resid 116  and name HG11))
   2 900     2 100     2 100 peak  6041 weight  0 11000E+01 volume  0.29943E+03 ppm1     8.086 ppm2     1.921
ASSI { 6051}
 (( segid "BrD " and resid 116  and name HN  ))
 (( segid "BrD " and resid 116  and name HG12))
   3 000     2 200     2 200 peak  6051 weight  0 11000E+01 volume  0 27021E+03 ppm1     8 083 ppm2     1.525
ASSI { 6061}
 (( segid "BrD " and resid 116  and name HN  ))
 (  segid "BrD " and resid 116  and name HG2%)
   2 500     1 600     1 600 peak  6061 weight  0 11000E+01 volume  0 86711E+03 ppm1     8 084 ppm2     1 420
ASSI { 6071}
 (( segid "BrD " and resid 110  and name HN  ))
 (( segid "BrD " and resid 110  and name HG12))
   3 000     2 200     2 200 peak  6071 weight  0 11000E+01 volume  0 25527E+03 ppm1     8 714 ppm2     1 679
ASSI { 6081}
 (( segid "BrD " and resid 110  and name HN  ))
 (  segid "BrD " and resid 110  and name HG2%)
   2 800     2 000     2 000 peak  6081 weight  0 11000E+01 volume  0 43268E+03 ppm1     8 714 ppm2     1 261
ASSI { 6091}
 (( segid "BrD " and resid 110  and name HN  ))
 (  segid "BrD " and resid 110  and name HD1%)
   3 400     2 900     2 100 peak  6091 weight  0.11000E+01 volume  0 13013E+03 ppm1     8 714 ppm2     1.116
ASSI { 6101}
 (( segid "BrD " and resid 50   and name HN  ))
 (( segid "BrD " and resid 50   and name HB  ))
   2 400     1 400     1 400 peak  6101 weight  0 11000E+01 volume  0 10564E+04 ppm1     8 564 ppm2     1 812
ASSI { 6111}
 (( segid "BrD " and resid 50   and name HN  ))
 (  segid "BrD " and resid 50   and name HD1%)
   3 200     2 600     2 300 peak  6111 weight  0 11000E+01 volume  0 17790E+03 ppm1     8 564 ppm2     1 144
ASSI { 6121}
 (( segid "BrD " and resid 50   and name HN  ))
 (( segid "BrD " and resid 50   and name HG12))
   3 300     2 700     2 200 peak  6121 weight  0 11000E+01 volume  0 13759E+03 ppm1     8 564 ppm2     0 823
ASSI { 6131}
 (( segid "BrD " and resid 50   and name HN  ))
 (  segid "BrD " and resid 50   and name HG2%)
   3 000     2 200     2 200 peak  6131 weight  0 11000E+01 volume  0 27674E+03 ppm1     8 564 ppm2     0 991
ASSI { 6141}
 (( segid "BrD " and resid 50   and name HN  ))
 (( segid "BrD " and resid 50   and name HG11))
   4 100     4 100     1 400 peak  6141 weight  0 11000E+01 volume  0 38065E+02 ppm1     8.564 ppm2     1 405
ASSI { 6151}
 (( segid "BrD " and resid 21   and name HN  ))
 (( segid "BrD " and resid 20   and name HB1 ))
   2 600     1 700     1 700 peak  6151 weight  0 11000E+01 volume  0 62145E+03 ppm1     8 544 ppm2     4 667
ASSI { 6161}
 (( segid "BrD " and resid 20   and name HN  ))
 (( segid "BrD " and resid 21   and name HN  ))
   2 800     2 000     2 000 peak  6161 weight  0 11000E+01 volume  0 39694E+03 ppm1     8 146 ppm2     8.547
ASSI { 6191}
 (( segid "BrD " and resid 22   and name HN  ))
 (( segid "BrD " and resid 21   and name HN  ))
   2 800     2 000     2 000 peak  6191 weight  0.11000E+01 volume  0 40962E+03 ppm1     9 455 ppm2     8 532
ASSI { 6201}
 (( segid "BrD " and resid 101  and name HN  ))
 (( segid "BrD " and resid 101  and name HG11))
   2 400     1 400     1 400 peak  6201 weight  0 11000E+01 volume  0 10700E+04 ppm1     8 514 ppm2     2 489
ASSI { 6211}
 (( segid "BrD " and resid 101  and name HN  ))
 (( segid "BrD " and resid 101  and name HG12))
   2 800     2 000     2 000 peak  6211 weight  0 11000E+01 volume  0 39771E+03 ppm1     8 513 ppm2     1 808
ASSI { 6221}
 (( segid "BrD " and resid 101  and name HN  ))
 (  segid "BrD " and resid 101  and name HG2%)
   2 700     1 800     1 800 peak  6221 weight  0 11000E+01 volume  0 49123E+03 ppm1     8 513 ppm2     1 596
ASSI { 6231}
 (( segid "BrD " and resid 21   and name HN  ))
 (( segid "BrD " and resid 21   and name HB  ))
   2.600     1.700     1 700 peak  6231 weight  0 11000E+01 volume  0.63964E+03 ppm1     8 545 ppm2     2 495
ASSI { 6241}
 (( segid "BrD " and resid 21   and name HN  ))
 (( segid "BrD " and resid 21   and name HG11))
   2 300     1.300     1 300 peak  6241 weight  0 11000E+01 volume  0 13646E+04 ppm1     8.545 ppm2     2 355
ASSI { 6251}
 (( segid "BrD " and resid 21   and name HN  ))
 (( segid "BrD " and resid 21   and name HG12))
   3 100     2 400     2 400 peak  6251 weight  0 11000E+01 volume  0 22794E+03 ppm1     8 556 ppm2     1 659
ASSI { 6261}
 (( segid "BrD " and resid 21   and name HN  ))
 (  segid "BrD " and resid 21   and name HG2%)
   2 600     1 700     1 700 peak  6261 weight  0 11000E+01 volume  0 60538E+03 ppm1     8 556 ppm2     1 605
ASSI { 6271}
 (( segid "BrD " and resid 21   and name HN  ))
 (  segid "BrD " and resid 21   and name HD1%)
   2 900     2 100     2 100 peak  6271 weight  0.11000E+01 volume  0 30098E+03 ppm1     8 545 ppm2     1 226
ASSI { 6281}
 (( segid "BrD " and resid 87   and name HN  ))
 (( segid "BrD " and resid 87   and name HB1 ))
   2.800     2.000     2 000 peak  6281 weight  0.11000E+01 volume  0.39163E+03 ppm1     8 570 ppm2     2 771
ASSI { 6291}
 (( segid "BrD " and resid 79   and name HN  ))
 (( segid "BrD " and resid 79   and name HB1 ))
   2 500     1 600     1 600 peak  6291 weight  0 11000E+01 volume  0 73947E+03 ppm1     8 681 ppm2     2.771
ASSI { 6301}
 (( segid "BrD " and resid 80   and name HN  ))
 (( segid "BrD " and resid 79   and name HB1 ))
   3.500     3 100     2.000 peak  6301 weight  0 11000E+01 volume  0 10437E+03 ppm1     8.006 ppm2     2 764
ASSI { 6311}
 (( segid "BrD " and resid 23   and name HN  ))
 (( segid "BrD " and resid 23   and name HG2 ))
   3 200     2 600     2 300 peak  6311 weight  0.11000E+01 volume  0 19029E+03 ppm1     9.120 ppm2     3 068
ASSI { 6321}
 (( segid "BrD " and resid 80   and name HN  ))
 (( segid "BrD " and resid 80   and name HG1 ))
   3 400     2 900     2 100 peak  6321 weight  0.11000E+01 volume  0 12866E+03 ppm1     8 006 ppm2     2 336
ASSI { 6331}
 (( segid "BrD " and resid 80   and name HN  ))
 (( segid "BrD " and resid 80   and name HB1 ))
   2 800     2 000     2 000 peak  6331 weight  0 11000E+01 volume  0 38416E+03 ppm1     8 006 ppm2     2 579
ASSI { 6341}
 (( segid "BrD " and resid 80   and name HN  ))
 (( segid "BrD " and resid 80   and name HB2 ))
   2 600     1 700     1 700 peak  6341 weight  0 11000E+01 volume  0 55298E+03 ppm1     8 006 ppm2     2.497
ASSI { 6351}
 (( segid "BrD " and resid 66   and name HN  ))
 (( segid "BrD " and resid 66   and name HB2 ))
   3 400     2.900     2 100 peak  6351 weight  0 11000E+01 volume  0 12971E+03 ppm1     8 763 ppm2     2.629
ASSI { 6361}
 (( segid "BrD " and resid 66   and name HN  ))
 (( segid "BrD " and resid 66   and name HG1 ))
   2 700     1 800     1 800 peak  6361 weight  0 11000E+01 volume  0 45372E+03 ppm1     8 764 ppm2     2 155
ASSI { 6371}
 (( segid "BrD " and resid 9    and name HN  ))
 (( segid "BrD " and resid 9    and name HG1 ))
   3 600     3 200     1 900 peak  6371 weight  0 11000E+01 volume  0 84495E+02 ppm1     9 053 ppm2     2 254
ASSI { 6381}
 (( segid "BrD " and resid 9    and name HN  ))
 (( segid "BrD " and resid 9    and name HB2 ))
   3 400     2 900     2 100 peak  6381 weight  0.11000E+01 volume  0 12497E+03 ppm1     9 055 ppm2     2 369
ASSI { 6391}
 (( segid "BrD " and resid 102  and name HN  ))
 (  segid "BrD " and resid 102  and name HD1%)
   3.100     2 400     2 400 peak  6391 weight  0 11000E+01 volume  0 19704E+03 ppm1     9 156 ppm2     1 310
ASSI { 6401}
 (( segid "BrD " and resid 102  and name HN  ))
 (( segid "BrD " and resid 102  and name HB2 ))
   2 400     1 400     1 400 peak  6401 weight  0 11000E+01 volume  0 88089E+03 ppm1     9 155 ppm2     1 808
ASSI { 6411}
 (( segid "BrD " and resid 102  and name HN  ))
 (( segid "BrD " and resid 102  and name HB1 ))
   2 700     1 800     1 800 peak  6411 weight  0.11000E+01 volume  0 47200E+03 ppm1     9 155 ppm2     2 002
ASSI { 6421}
 (( segid "BrD " and resid 102  and name HN  ))
 (( segid "BrD " and resid 102  and name HG  ))
   3 200     2 600     2 300 peak  6421 weight  0.11000E+01 volume  0 16630E+03 ppm1     9 157 ppm2     2 152
ASSI { 6431}
 (( segid "BrD " and resid 73   and name HN  ))
 (( segid "BrD " and resid 73   and name HB2 ))
   2 800     2 000     2 000 peak  6431 weight  0.11000E+01 volume  0 37491E+03 ppm1     8 045 ppm2     2 495
ASSI { 6441}
 (( segid "BrD " and resid 73   and name HN  ))
 (( segid "BrD " and resid 73   and name HG  ))
   3 400     2.900     2 100 peak  6441 weight  0 11000E+01 volume  0 13407E+03 ppm1     8 045 ppm2     2 376
ASSI { 6451}
 (( segid "BrD " and resid 73   and name HN  ))
 (  segid "BrD " and resid 73   and name HD2%)
   3 600     3.200     1 900 peak  6451 weight  0 11000E+01 volume  0 91167E+02 ppm1     8 049 ppm2     1.491
ASSI { 6461}
 (( segid "BrD " and resid 56   and name HN  ))
 (  segid "BrD " and resid 56   and name HD1%)
   3 200     2 600     2 300 peak  6461 weight  0 11000E+01 volume  0 17282E+03 ppm1     9 679 ppm2     1 521
ASSI { 6471}
 (( segid "BrD " and resid 56   and name HN  ))
 (( segid "BrD " and resid 56   and name HG  ))
   2 500     1 600     1 600 peak  6471 weight  0.11000E+01 volume  0 74688E+03 ppm1     9 680 ppm2     2.320
ASSI { 6481}
 (( segid "BrD " and resid 56   and name HN  ))
 (( segid "BrD " and resid 56   and name HB2 ))
   3 100     2.400     2 400 peak  6481 weight  0 11000E+01 volume  0 21719E+03 ppm1     9 680 ppm2     2 002
ASSI { 6491}
 (( segid "BrD " and resid 22   and name HN  ))
 (  segid "BrD " and resid 22   and name HD1%)
   3.200     2 600     2 300 peak  6491 weight  0 11000E+01 volume  0 16857E+03 ppm1     9 456 ppm2     1 668
ASSI { 6501}
 (( segid "BrD " and resid 22   and name HN  ))
 (( segid "BrD " and resid 22   and name HB2 ))
   2 400     1 400     1 400 peak  6501 weight  0 11000E+01 volume  0 10653E+04 ppm1     9 455 ppm2     2 292
ASSI { 6511}
 (( segid "BrD " and resid 22   and name HN  ))
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(( segid "BrD " and resid 22   and name HB1 ))
   2 700     1.800     1 800 peak  6511 weight  0 11000E+01 volume  0 47530E+03 ppm1     9 455 ppm2     2.693
ASSI { 6521}
  (( segid "BrD " and resid 22   and name HN  ))
  (( segid "BrD " and resid 22   and name HG  ))
   3 700     3 400     1 800 peak  6521 weight  0 11000E+01 volume  0 69056E+02 ppm1     9 455 ppm2     2 366
ASSI { 6531}
  (( segid "BrD " and resid 63   and name HN  ))
  (  segid "BrD " and resid 63   and name HD2%)
   3 200     2 600     2 300 peak  6531 weight  0 11000E+01 volume  0 19269E+03 ppm1     9.473 ppm2     1 478
ASSI { 6541}
  (( segid "BrD " and resid 63   and name HN  ))
  (  segid "BrD " and resid 63   and name HD1%)
   3 100     2 400     2 400 peak  6541 weight  0 11000E+01 volume  0 21627E+03 ppm1     9 472 ppm2     1 674
ASSI { 6561}
  (( segid "BrD " and resid 63   and name HN  ))
  (( segid "BrD " and resid 63   and name HB2 ))
   2 500     1.600     1 600 peak  6561 weight  0 11000E+01 volume  0 86099E+03 ppm1     9 473 ppm2     2 532
ASSI { 6571}
  (( segid "BrD " and resid 63   and name HN  ))
  (( segid "BrD " and resid 63   and name HG  ))
   3 000     2 200     2 200 peak  6571 weight  0 11000E+01 volume  0 26899E+03 ppm1     9 472 ppm2     2 439
ASSI { 6581}
  (( segid "BrD " and resid 14   and name HN  ))
  (( segid "BrD " and resid 14   and name HB1 ))
   2 500     1 600     1 600 peak  6581 weight  0.11000E+01 volume  0 80229E+03 ppm1     8 809 ppm2     2 453
ASSI { 6591}
  (( segid "BrD " and resid 14   and name HN  ))
  (( segid "BrD " and resid 14   and name HG  ))
   3 000     2.200     2 200 peak  6591 weight  0 11000E+01 volume  0 24747E+03 ppm1     8 809 ppm2     2 064
ASSI { 6601}
  (( segid "BrD " and resid 14   and name HN  ))
  (( segid "BrD " and resid 14   and name HB2 ))
   2 500     1 600     1.600 peak  6601 weight  0 11000E+01 volume  0.85081E+03 ppm1     8.809 ppm2     2 164
ASSI { 6611}
  (( segid "BrD " and resid 14   and name HN  ))
  (  segid "BrD " and resid 14   and name HD1%)
   3 200     2 600     2 300 peak  6611 weight  0 11000E+01 volume  0 18673E+03 ppm1     8 809 ppm2     1.401
ASSI { 6621}
  (( segid "BrD " and resid 24   and name HN  ))
  (( segid "BrD " and resid 24   and name HG2 ))
   2 300     1 300     1.300 peak  6621 weight  0 11000E+01 volume  0 12087E+04 ppm1     8 654 ppm2     3 032
ASSI { 6631}  .
  (( segid "BrD " and resid 49   and name HN  ))
  (  segid "BrD " and resid 49   and name HG1%)
   3 100     2 400     2 400 peak  6631 weight  0 11000E+01 volume  0 20533E+03 ppm1     7 762 ppm2     1 652
ASSI { 6641}
  (( segid "BrD " and resid 50   and name HN  ))
  (  segid "BrD " and resid 49   and name HG1%)
   3 400     2 900     2 100 peak  6641 weight  0 11000E+01 volume  0 12406E+03 ppm1     8 564 ppm2     1 652
ASSI { 6651}
  (( segid "BrD " and resid 64   and name HN  ))
  (( segid "BrD " and resid 64   and name HB1 ))
   2 400     1 400     1 400 peak  6651 weight  0 11000E+01 volume  0 10941E+04 ppm1     8 584 ppm2     2 661
ASSI { 6661}
  (( segid "BrD " and resid 64   and name HN  ))
  (( segid "BrD " and resid 64   and name HG1 ))
   2 700     1 800     1.800 peak  6661 weight  0 11000E+01 volume  0 45034E+03 ppm1     8.584 ppm2     2 210
ASSI { 6671}
  (( segid "BrD " and resid 64   and name HN  ))
  (( segid "BrD " and resid 64   and name HD1 ))
   3 600     3 200     1 900 peak  6671 weight  0 11000E+01 volume  0 82950E+02 ppm1     8 584 ppm2     2 411
ASSI { 6681}
  (( segid "BrD " and resid 104  and name HN  ))
  (( segid "BrD " and resid 104  and name HB1 ))
   2 600     1 700     1 700 peak  6681 weight  0 11000E+01 volume  0 59758E+03 ppm1     7 763 ppm2     2 537
ASSI { 6691}
  (( segid "BrD " and resid 104  and name HN  ))
  (( segid "BrD " and resid 104  and name HG1 ))
   3 000     2 200     2.200 peak  6691 weight  0 11000E+01 volume  0 24911E+03 ppm1     7 763 ppm2     2.099
ASSI { 6701}
  (( segid "BrD " and resid 104  and name HN  ))
  (( segid "BrD " and resid 104  and name HD1 ))
   2 900     2 100     2 100 peak  6701 weight  0 11000E+01 volume  0.30408E+03 ppm1     7 763 ppm2     2.288
ASSI { 6711}
  (( segid "BrD " and resid 111  and name HN  ))
  (( segid "BrD " and resid 111  and name HB1 ))
   2 600     1 700     1 700 peak  6711 weight  0 11000E+01 volume  0.66813E+03 ppm1     8 168 ppm2     2 482
ASSI { 6721}
  (( segid "BrD " and resid 111  and name HN  ))
  (( segid "BrD " and resid 111  and name HB2 ))
   2 400     1 400     1.400 peak  6721 weight  0 11000E+01 volume  0 98067E+03 ppm1     8.170 ppm2     2.376
ASSI { 6731}
  (( segid "BrD " and resid 111  and name HN  ))
  (( segid "BrD " and resid 111  and name HG2 ))
   3 600     3.200     1.900 peak  6731 weight  0 11000E+01 volume  0 88731E+02 ppm1     8 168 ppm2     1.922
ASSI { 6741}
  (( segid "BrD " and resid 111  and name HN  ))
  (( segid "BrD " and resid 111  and name HG1 ))
   3 200     2 600     2 300 peak  6741 weight  0 11000E+01 volume  0.16392E+03 ppm1     8 168 ppm2     2 002
ASSI { 6761}
  (( segid "BrD " and resid 19   and name HN  ))
  (( segid "BrD " and resid 19   and name HB1 ))
   2.700     1 800     1 800 peak  6761 weight  0 11000E+01 volume  0 53478E+03 ppm1     9 187 ppm2     2 325
ASSI { 6771}
  (( segid "BrD " and resid 19   and name HN  ))
  (( segid "BrD " and resid 19   and name HG1 ))
   4 000     4 000     1 500 peak  6771 weight  0.11000E+01 volume  0 45358E+02 ppm1     9 188 ppm2     1 879
ASSI { 6781}
  (( segid "BrD " and resid 19   and name HN  ))
  (( segid "BrD " and resid 18   and name HG  ))
   2 800     2 000     2 000 peak  6781 weight  0 11000E+01 volume  0 38484E+03 ppm1     9 187 ppm2     2 271
ASSI { 6791}
  (( segid "BrD " and resid 12   and name HN  ))
  (( segid "BrD " and resid 11   and name HA  ))
   3 000     2.200     2 200 peak  6791 weight  0 11000E+01 volume  0.26617E+03 ppm1     9 021 ppm2     4 940
ASSI { 6801}
  (( segid "BrD " and resid 97   and name HN  ))
  (( segid "BrD " and resid 97   and name HB1 ))
   2.300     1.300     1 300 peak  6801 weight  0 11000E+01 volume  0 12859E+04 ppm1     8 674 ppm2     2 708
ASSI { 6811}
  (( segid "BrD " and resid 97   and name HN  ))
  (( segid "BrD " and resid 97   and name HG2 ))
   2 900     2 100     2 100 peak  6811 weight  0 11000E+01 volume  0 32919E+03 ppm1     8 674 ppm2     2.193
ASSI { 6821}
  (( segid "BrD " and resid 109  and name HN  ))
  (( segid "BrD " and resid 109  and name HB1 ))
   2 300     1 300     1 300 peak  6821 weight  0 11000E+01 volume  0 11797E+04 ppm1     8 573 ppm2     2.336
ASSI { 6831}
  (( segid "BrD " and resid 109  and name HN  ))
  (( segid "BrD " and resid 109  and name HB2 ))
   3 200     2 600     2 300 peak  6831 weight  0 11000E+01 volume  0 19151E+03 ppm1     8 573 ppm2     2 173
ASSI { 6841}
  (( segid "BrD " and resid 109  and name HN  ))
  (( segid "BrD " and resid 109  and name HG1 ))
   3.700     3 400     1 800 peak  6841 weight  0 11000E+01 volume  0 70793E+02 ppm1     8.574 ppm2     1.439
ASSI { 6881}
  (( segid "BrD " and resid 86   and name HN  ))
  (( segid "BrD " and resid 86   and name HB1 ))
   2 700     1 800     1 800 peak  6881 weight  0 11000E+01 volume  0 51142E+03 ppm1     8 422 ppm2     2.359
ASSI { 6891}
  (( segid "BrD " and resid 86   and name HN  ))
  (( segid "BrD " and resid 86   and name HG2 ))
   3 400     2 900     2 100 peak  6891 weight  0.11000E+01 volume  0 13112E+03 ppm1     8 423 ppm2     0 745
ASSI { 6901}
  (( segid "BrD " and resid 86   and name HN  ))
  (( segid "BrD " and resid 86   and name HD1 ))
   3.800     3.600     1 700 peak  6901 weight  0 11000E+01 volume  0 59192E+02 ppm1     8 423 ppm2     1 862
ASSI { 6921}
  (( segid "BrD " and resid 103  and name HN  ))
  (( segid "BrD " and resid 103  and name HG1 ))
   3 000     2 200     2 200 peak  6921 weight  0 11000E+01 volume  0 24153E+03 ppm1     8 695 ppm2     2 613
ASSI { 6931}
  (( segid "BrD " and resid 104  and name HN  ))
  (( segid "BrD " and resid 103  and name HG1 ))
   3 200     2 600     2 300 peak  6931 weight  0 11000E+01 volume  0 18108E+03 ppm1     7 763 ppm2     2 608
ASSI { 6941}
  (( segid "BrD " and resid 48   and name HN  ))
  (( segid "BrD " and resid 48   and name HG1 ))
   3 300     2.700     2.200 peak  6941 weight  0.11000E+01 volume  0 14027E+03 ppm1     8.307 ppm2     2 909
ASSI { 6951}
  (( segid "BrD " and resid 49   and name HN  ))
  (( segid "BrD " and resid 48   and name HG1 ))
   4 100     4 100     1 400 peak  6951 weight  0.11000E+01 volume  0.41580E+02 ppm1     7.762 ppm2     2.932
ASSI { 6961}
  (( segid "BrD " and resid 66   and name HN  ))
  (( segid "BrD " and resid 66   and name HB1 ))
   3 200     2 600     2 300 peak  6961 weight  0 11000E+01 volume  0 17814E+03 ppm1     8 763 ppm2     2 704
ASSI { 6971}
  (( segid "BrD " and resid 35   and name HN  ))
  (( segid "BrD " and resid 35   and name HB1 ))
   2.900     2.100     2 100 peak  6971 weight  0.11000E+01 volume  0 32270E+03 ppm1     7 734 ppm2     2 850
ASSI { 6981}
  (( segid "BrD " and resid 54   and name HN  ))
  (( segid "BrD " and resid 53   and name HA  ))
   2.500     1 600     1 600 peak  6981 weight  0 11000E+01 volume  0 78564E+03 ppm1     9 036 ppm2     4 690
ASSI { 6991}
  (( segid "BrD " and resid 38   and name HN  ))
  (( segid "BrD " and resid 37   and name HA  ))
   2 200     1 200     1 200 peak  6991 weight  0 11000E+01 volume  0 16736E+04 ppm1     8 731 ppm2     4 849
ASSI { 7001}
  (( segid "BrD " and resid 51   and name HN  ))
  (( segid "BrD " and resid 51   and name HB1 ))
   2.900     2 100     2 100 peak  7001 weight  0 11000E+01 volume  0 35413E+03 ppm1     8 375 ppm2     1 980
ASSI { 7011}
  (( segid "BrD " and resid 51   and name HN  ))
  (( segid "BrD " and resid 51   and name HB2 ))
   3 000     2.200     2.200 peak  7011 weight  0.11000E+01 volume  0 24666E+03 ppm1     8 375 ppm2     1 818
ASSI { 7021}
  (( segid "BrD " and resid 51   and name HN  ))
  (( segid "BrD " and resid 51   and name HG2 ))
   3 000     2 200     2 200 peak  7021 weight  0.11000E+01 volume  0 24666E+03 ppm1     8.375 ppm2     1 786
ASSI { 7041}
  (( segid "BrD " and resid 52   and name HN  ))
  (( segid "BrD " and resid 52   and name HA  ))
   2 900     2 100     2 100 peak  7041 weight  0 11000E+01 volume  0 32203E+03 ppm1     9 004 ppm2     5 591
ASSI { 7051}
  (( segid "BrD " and resid 52   and name HN  ))
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   (( segid "BrD " and resid 52   and name HB1 ))
     2.700     1.800     1.800 peak  7051 weight  0.11000E+01 volume  0.48728E+03 ppm1     9.004 ppm2     3.641
ASSI { 7061}
   (( segid "BrD " and resid 52   and name HN  ))
   (( segid "BrD " and resid 52   and name HB2 ))
     2 500     1 600     1 600 peak  7061 weight  0 11000E+01 volume  0 72550E+03 ppm1     9.003 ppm2     3 514
ASSI { 7071}
   (( segid "BrD " and resid 52   and name HN  ))
   (( segid "BrD " and resid 51   and name HN  ))
     2 600     1 700     1 700 peak  7071 weight  0 11000E+01 volume  0 63507E+03 ppm1     9.004 ppm2     8 356
ASSI { 7091}
   (( segid "BrD " and resid 52   and name HN  ))
   (( segid "BrD " and resid 51   and name HA  ))
     3.000     2 200     2 200 peak  7091 weight  0 11000E+01 volume  0 26640E+03 ppm1     9 004 ppm2     4 482
ASSI { 7101}
   (( segid "BrD " and resid 52   and name HN  ))
   (( segid "BrD " and resid 53   and name HD1 ))
     3.500     3 100     2 000 peak  7101 weight  0 11000E+01 volume  0 10263E+03 ppm1     9 004 ppm2     4 230
ASSI { 7111}
   (( segid "BrD " and resid 52   and name HN  ))
   (( segid "BrD " and resid 53   and name HD2 ))
     3 900     3 800     1 600 peak  7111 weight  0 11000E+01 volume  0 57287E+02 ppm1     9 003 ppm2     3 997
ASSI { 7141}
   (( segid "BrD " and resid 59   and name HN  ))
   (( segid "BrD " and resid 59   and name HG2 ))
     3 300     2 700     2 200 peak  7141 weight  0 11000E+01 volume  0 14988E+03 ppm1     8.496 ppm2     3 103
ASSI { 7151}
   (( segid "BrD " and resid 59   and name HN  ))
   (( segid "BrD " and resid 59   and name HG1 ))
     3 400     2 900     2 100 peak  7151 weight  0 11000E+01 volume  0 12335E+03 ppm1     8 498 ppm2     3 228
ASSI { 7161}
   (( segid "BrD " and resid 59   and name HN  ))
   (( segid "BrD " and resid 59   and name HB1 ))
     3 400     2.900     2 100 peak  7161 weight  0 11000E+01 volume  0 11956E+03 ppm1     8.498 ppm2     2 700
ASSI { 7171}
   (( segid "BrD " and resid 59   and name HN  ))
   (( segid "BrD " and resid 59   and name HB2 ))
     3 200     2 600     2 300 peak  7171 weight  0 11000E+01 volume  0 17215E+03 ppm1     8 499 ppm2     2 504
ASSI { 7181}
   (( segid "BrD " and resid 57   and name HN  ))
   (( segid "BrD " and resid 57   and name HB1 ))
     2 400     1.400     1 400 peak  7181 weight  0 11000E+01 volume  0 94732E+03 ppm1     9 359 ppm2     2 947
ASSI { 7191}
   (( segid "BrD " and resid 57   and name HN  ))
   (( segid "BrD " and resid 57   and name HB2 ))
     2 500     1 600     1 600 peak  7191 weight  0 11000E+01 volume  0 75718E+03 ppm1     9 358 ppm2     2 827
ASSI { 7201}
   (( segid "BrD " and resid 57   and name HN  ))
   (( segid "BrD " and resid 57   and name HG1 ))
     3 600     3 200     1 900 peak  7201 weight  0 11000E+01 volume  0 93147E+02 ppm1     9 359 ppm2     2 088
ASSI { 7211}
   (( segid "BrD " and resid 57   and name HN  ))
   (( segid "BrD " and resid 57   and name HD1 ))
     4 300     4 300     1 200 peak  7211 weight  0 11000E+01 volume  0 28923E+02 ppm1     9 358 ppm2     2 411
ASSI { 7221}
   (( segid "BrD " and resid 57   and name HN  ))
   (( segid "BrD " and resid 57   and name HD2 ))
     3 400     2 900     2 100 peak  7221 weight  0 11000E+01 volume  0 13023E+03 ppm1     9 359 ppm2     2 292
ASSI { 7231}
   (( segid "BrD " and resid 26   and name HN  ))
   (( segid "BrD " and resid 26   and name HB1 ))
     3 300     2 700     2 200 peak  7231 weight  0.11000E+01 volume  0 15703E+03 ppm1     9 195 ppm2     2 463
ASSI { 7241}
   (( segid "BrD " and resid 26   and name HN  ))
   (( segid "BrD " and resid 26   and name HD1 ))
     3.500     3 100     2 000 peak  7241 weight  0 11000E+01 volume  0 99010E+02 ppm1     9 196 ppm2     2 092
ASSI { 7261}
   (( segid "BrD " and resid 10   and name HN  ))
   (( segid "BrD " and resid 11   and name HD1 ))
     4 600     4 600     0 900 peak  7261 weight  0 11000E+01 volume  0 20621E+02 ppm1     8 885 ppm2     4 475
ASSI { 7271}
   (( segid "BrD " and resid 10   and name HN  ))
   (( segid "BrD " and resid 9    and name HB1 ))
     3 400     2 900     2 100 peak  7271 weight  0 11000E+01 volume  0 12456E+03 ppm1     8 883 ppm2     2 422
ASSI { 7281}
   (( segid "BrD " and resid 13   and name HN  ))
   (( segid "BrD " and resid 12   and name HB1 ))
     3 500     3 100     2 000 peak  7281 weight  0 11000E+01 volume  0 11107E+03 ppm1     8.802 ppm2     3 399
ASSI { 7301}
   (( segid "BrD " and resid 15   and name HN  ))
   (( segid "BrD " and resid 14   and name HN  ))
     2 900     2 100     2 100 peak  7301 weight  0.11000E+01 volume  0 28889E+03 ppm1     8 597 ppm2     8 817
ASSI { 7311}
   (( segid "BrD " and resid 16   and name HN  ))
   (( segid "BrD " and resid 13   and name HA  ))
     3.500     3 100     2.000 peak  7311 weight  0 11000E+01 volume  0 96679E+02 ppm1     8 794 ppm2     4 770
ASSI { 7321}
   (( segid "BrD " and resid 15   and name HN  ))
   (  segid "BrD " and resid 14   and name HD2%)
     3 600     3.200     1 900 peak  7321 weight  0 11000E+01 volume  0 89979E+02 ppm1     8 598 ppm2     1 393
ASSI { 7331}
   (( segid "BrD " and resid 15   and name HN  ))
   (( segid "BrD " and resid 14   and name HB1 ))
     2 600     1 700     1 700 peak  7331 weight  0 11000E+01 volume  0 55160E+03 ppm1     8 599 ppm2     2.454
ASSI { 7341}
   (( segid "BrD " and resid 15   and name HN  ))
   (( segid "BrD " and resid 14   and name HB2 ))
     3 600     3 200     1 900 peak  7341 weight  0 11000E+01 volume  0 85197E+02 ppm1     8 598 ppm2     2 162
ASSI { 7351}
   (( segid "BrD " and resid 18   and name HN  ))
   (( segid "BrD " and resid 14   and name HA  ))
     3 500     3 100     2 000 peak  7351 weight  0 11000E+01 volume  0 10770E+03 ppm1     9 071 ppm2     4 652
ASSI { 7361}
   (( segid "BrD " and resid 21   and name HN  ))
   (( segid "BrD " and resid 18   and name HA  ))
     3 200     2 600     2.300 peak  7361 weight  0.11000E+01 volume  0.16933E+03 ppm1     8 544 ppm2     3 874
ASSI { 7371}
   (( segid "BrD " and resid 22   and name HN  ))
   (( segid "BrD " and resid 18   and name HA  ))
     3 700     3 400     1 800 peak  7371 weight  0 11000E+01 volume  0 72924E+02 ppm1     9 456 ppm2     3 896
ASSI { 7381}
   (( segid "BrD " and resid 19   and name HN  ))
   (( segid "BrD " and resid 18   and name HB1 ))
     2 800     2 000     2 000 peak  7381 weight  0 11000E+01 volume  0 40235E+03 ppm1     9 186 ppm2     2 139
ASSI { 7391}
   (( segid "BrD " and resid 19   and name HN  ))
   (  segid "BrD " and resid 18   and name HD1%)
     3 800     3 600     1 700 peak  7391 weight  0 11000E+01 volume  0 63600E+02 ppm1     9 189 ppm2     1 084
ASSI { 7401}
   (( segid "BrD " and resid 19   and name HN  ))
   (  segid "BrD " and resid 18   and name HD2%)
     3 700     3 400     1 800 peak  7401 weight  0 11000E+01 volume  0 71915E+02 ppm1     9 187 ppm2     0 414
ASSI { 7411}
   (( segid "BrD " and resid 20   and name HN  ))
   (( segid "BrD " and resid 19   and name HB1 ))
     3 200     2 600     2 300 peak  7411 weight  0 11000E+01 volume  0 16507E+03 ppm1     8 146 ppm2     2 336
ASSI { 7421}
   (( segid "BrD " and resid 20   and name HN  ))
   (( segid "BrD " and resid 19   and name HB2 ))
     3 400     2 900     2 100 peak  7421 weight  0 11000E+01 volume  0 13044E+03 ppm1     8 147 ppm2     1 967
ASSI { 7431}
   (( segid "BrD " and resid 23   and name HN  ))
   (( segid "BrD " and resid 19   and name HA  ))
     3 600     3 200     1 900 peak  7431 weight  0.11000E+01 volume  0 90645E+02 ppm1     9 120 ppm2     4 286
ASSI { 7441}
   (( segid "BrD " and resid 23   and name HN  ))
   (( segid "BrD " and resid 20   and name HA  ))
     3 400     2 900     2 100 peak  7441 weight  0 11000E+01 volume  0 11524E+03 ppm1     9 118 ppm2     4 895
ASSI { 7451}
   (( segid "BrD " and resid 20   and name HN  ))
   (( segid "BrD " and resid 22   and name HN  ))
     3 600     3 200     1 900 peak  7451 weight  0 11000E+01 volume  0 81392E+02 ppm1     8.147 ppm2     9 450
ASSI { 7471}
   (( segid "BrD " and resid 21   and name HN  ))
   (( segid "BrD " and resid 23   and name HN  ))
     4.100     4 100     1 400 peak  7471 weight  0 11000E+01 volume  0 42834E+02 ppm1     8 545 ppm2     9 130
ASSI { 7491}
   (( segid "BrD " and resid 24   and name HN  ))
   (( segid "BrD " and resid 21   and name HA  ))
     3.200     2 600     2 300 peak  7491 weight  0 11000E+01 volume  0 16448E+03 ppm1     8 661 ppm2     4 371
ASSI { 7501}
   (( segid "BrD " and resid 26   and name HN  ))
   (( segid "BrD " and resid 23   and name HA  ))
     3.400     2 900     2 100 peak  7501 weight  0 11000E+01 volume  0 12059E+03 ppm1     9 196 ppm2     4 639
ASSI { 7511}
   (( segid "BrD " and resid 27   and name HN  ))
   (( segid "BrD " and resid 24   and name HA  ))
     3 200     2 600     2 300 peak  7511 weight  0 11000E+01 volume  0 17746E+03 ppm1     8 170 ppm2     4 777
ASSI { 7521}
   (( segid "BrD " and resid 28   and name HN  ))
   (( segid "BrD " and resid 25   and name HA  ))
     3 600     3 200     1 900 peak  7521 weight  0 11000E+01 volume  0 92661E+02 ppm1     8.166 ppm2     4 449
ASSI { 7531}
   (( segid "BrD " and resid 26   and name HN  ))
   (( segid "BrD " and resid 25   and name HB  ))
     2.600     1.700     1 700 peak  7531 weight  0 11000E+01 volume  0.67212E+03 ppm1     9 196 ppm2     2 991
ASSI { 7541}
   (( segid "BrD " and resid 26   and name HN  ))
   (  segid "BrD " and resid 25   and name HG2%)
     2 900     2.100     2 100 peak  7541 weight  0 11000E+01 volume  0.31151E+03 ppm1     9 196 ppm2     1 640
ASSI { 7551}
   (( segid "BrD " and resid 26   and name HN  ))
   (  segid "BrD " and resid 25   and name HG1%)
     3 100     2.400     2 400 peak  7551 weight  0.11000E+01 volume  0 21302E+03 ppm1     9 197 ppm2     1 790
ASSI { 7561}
   (( segid "BrD " and resid 43   and name HN  ))
   (( segid "BrD " and resid 44   and name HD1 ))
     3 400     2 900     2 100 peak  7561 weight  0 11000E+01 volume  0 11281E+03 ppm1     8.001 ppm2     4.324
ASSI { 7571}
   (( segid "BrD " and resid 43   and name HN  ))
   (( segid "BrD " and resid 44   and name HD2 ))
     3 100     2 400     2 400 peak  7571 weight  0 11000E+01 volume  0 21754E+03 ppm1     8 001 ppm2     4.122
ASSI { 7581}
   (( segid "BrD " and resid 49   and name HN  ))
   (( segid "BrD " and resid 46   and name HA  ))
     3.900     3 800     1 600 peak  7581 weight  0 11000E+01 volume  0 54216E+02 ppm1     7 763 ppm2     4 143
ASSI { 7591}
   (( segid "BrD " and resid 56   and name HN  ))
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(( segid "BrD " and resid 56   and name HB1 ))
  2.700    1.800    1 800 peak  7591 weight  0 11000E+01 volume  0 48254E+03 ppm1    9 679 ppm2    2 693
ASSI { 7601}
 (( segid "BrD " and resid 61   and name HN  ))
 (( segid "BrD " and resid 58   and name HA  ))
  2 900    2 100    2 100 peak  7601 weight  0 11000E+01 volume  0 30089E+03 ppm1    8 749 ppm2    4 452
ASSI { 7611}
 (( segid "BrD " and resid 64   and name HN  ))
 (( segid "BrD " and resid 60   and name HA  ))
  3 400    2 900    2 100 peak  7611 weight  0 11000E+01 volume  0 11932E+03 ppm1    8 584 ppm2    4 807
ASSI { 7621}
 (( segid "BrD " and resid 66   and name HN  ))
 (( segid "BrD " and resid 66   and name HD1 ))
  2 900    2 100    2 100 peak  7621 weight  0 11000E+01 volume  0.29994E+03 ppm1    8 759 ppm2    3 667
ASSI { 7631}
 (( segid "BrD " and resid 75   and name HN  ))
 (( segid "BrD " and resid 72   and name HA  ))
  3 400    2 900    2 100 peak  7631 weight  0 11000E+01 volume  0.13400E+03 ppm1    9 106 ppm2    4 669
ASSI { 7651}
 (( segid "BrD " and resid 79   and name HN  ))
 (( segid "BrD " and resid 76   and name HA  ))
  3 200    2 600    2 300 peak  7651 weight  0 11000E+01 volume  0.16410E+03 ppm1    8.680 ppm2    4 691
ASSI { 7661}
 (( segid "BrD " and resid 80   and name HN  ))
 (( segid "BrD " and resid 77   and name HA  ))
  3 700    3 400    1 800 peak  7661 weight  0 11000E+01 volume  0 79484E+02 ppm1    8 006 ppm2    4 969
ASSI { 7671}
 (( segid "BrD " and resid 81   and name HN  ))
 (( segid "BrD " and resid 78   and name HA  ))
  3 300    2 700    2 200 peak  7671 weight  0 11000E+01 volume  0 15049E+03 ppm1    7 639 ppm2    3 989
ASSI { 7681}
 (( segid "BrD " and resid 82   and name HN  ))
 (( segid "BrD " and resid 79   and name HA  ))
  3 600    3 200    1 900 peak  7681 weight  0 11000E+01 volume  0 80779E+02 ppm1    6 981 ppm2    4 411
ASSI { 7701}
 (( segid "BrD " and resid 84   and name HN  ))
 (( segid "BrD " and resid 81   and name HA  ))
  3 500    3 100    2 000 peak  7701 weight  0 11000E+01 volume  0 10576E+03 ppm1    9 463 ppm2    3 705
ASSI { 7711}
 (( segid "BrD " and resid 85   and name HN  ))
 (( segid "BrD " and resid 82   and name HA  ))
  3 300    2 700    2 200 peak  7711 weight  0 11000E+01 volume  0 13652E+03 ppm1    7 516 ppm2    4 768
ASSI { 7721}
 (( segid "BrD " and resid 89   and name HN  ))
 (( segid "BrD " and resid 86   and name HA  ))
  3 500    3 100    2 000 peak  7721 weight  0 11000E+01 volume  0 10495E+03 ppm1    8 858 ppm2    4 811
ASSI { 7731}
 (( segid "BrD " and resid 93   and name HN  ))
 (( segid "BrD " and resid 92   and name HA  ))
  3 600    3 200    1 900 peak  7731 weight  0 11000E+01 volume  0 94491E+02 ppm1    8.713 ppm2    4 796
ASSI { 7741}
 (( segid "BrD " and resid 98   and name HN  ))
 (( segid "BrD " and resid 95   and name HA  ))
  3 300    2 700    2 200 peak  7741 weight  0 11000E+01 volume  0 14245E+03 ppm1    9 125 ppm2    4 441
ASSI { 7751}
 (( segid "BrD " and resid 77   and name HN  ))
 (( segid "BrD " and resid 75   and name HN  ))
  3 500    3 100    2 000 peak  7751 weight  0 11000E+01 volume  0 10255E+03 ppm1    7.985 ppm2    9 096
ASSI { 7761}
 (( segid "BrD " and resid 98   and name HN  ))
 (( segid "BrD " and resid 96   and name HN  ))
  3 900    3 800    1 600 peak  7761 weight  0.11000E+01 volume  0 51137E+02 ppm1    9 125 ppm2    7 963
ASSI { 7771}
 (( segid "BrD " and resid 102  and name HN  ))
 (( segid "BrD " and resid 98   and name HA  ))
  3 500    3 100    2.000 peak  7771 weight  0 11000E+01 volume  0.10795E+03 ppm1    9 156 ppm2    4 809
ASSI { 7781}
 (( segid "BrD " and resid 102  and name HN  ))
 (( segid "BrD " and resid 99   and name HA  ))
  3 500    3 100    2 000 peak  7781 weight  0 11000E+01 volume  0.10223E+03 ppm1    9 156 ppm2    4 443
ASSI { 7791}
 (( segid "BrD " and resid 103  and name HN  ))
 (( segid "BrD " and resid 100  and name HA  ))
  3 000    2 200    2 200 peak  7791 weight  0 11000E+01 volume  0.26822E+03 ppm1    8 696 ppm2    4 932
ASSI { 7801}
 (( segid "BrD " and resid 104  and name HN  ))
 (( segid "BrD " and resid 101  and name HA  ))
  3 000    2 200    2 200 peak  7801 weight  0 11000E+01 volume  0 25521E+03 ppm1    7 763 ppm2    4 275
ASSI { 7811}
 (( segid "BrD " and resid 102  and name HN  ))
 (( segid "BrD " and resid 104  and name HN  ))
  4 300    4 300    1.200 peak  7811 weight  0 11000E+01 volume  0 28976E+02 ppm1    9 156 ppm2    7 772
ASSI { 7831}
 (( segid "BrD " and resid 105  and name HN  ))
 (( segid "BrD " and resid 102  and name HA  ))
  3 300    2 700    2 200 peak  7831 weight  0 11000E+01 volume  0 14640E+03 ppm1    8 488 ppm2    4 290
ASSI { 7841}
 (( segid "BrD " and resid 108  and name HN  ))
 (( segid "BrD " and resid 105  and name HA  ))
  3.600    3 200    1 900 peak  7841 weight  0 11000E+01 volume  0 82783E+02 ppm1    8 526 ppm2    4 936
ASSI { 7851}
 (( segid "BrD " and resid 16   and name HN  ))
 (( segid "BrD " and resid 16   and name HB1 ))
  2 900    2 100    2 100 peak  7851 weight  0 11000E+01 volume  0 35014E+03 ppm1    8 794 ppm2    4 587
ASSI { 7861}
 (( segid "BrD " and resid 24   and name HE22))
 (( segid "BrD " and resid 24   and name HG2 ))
  4 100    4 100    1 400 peak  7861 weight  0 11000E+01 volume  0.40620E+02 ppm1    7 523 ppm2    3 068
ASSI { 7871}
 (( segid "BrD " and resid 24   and name HE21))
 (( segid "BrD " and resid 24   and name HG2 ))
  3 500    3.100    2 000 peak  7871 weight  0 11000E+01 volume  0 10084E+03 ppm1    7 629 ppm2    3 067
ASSI { 7881}
 (( segid "BrD " and resid 25   and name HN  ))
 (( segid "BrD " and resid 24   and name HG1 ))
  3 400    2 900    2 100 peak  7881 weight  0 11000E+01 volume  0 11666E+03 ppm1    9 133 ppm2    3.447
ASSI { 7891}
 (( segid "BrD " and resid 18   and name HN  ))
 (  segid "BrD " and resid 18   and name HD1%)
  2 900    2 100    2 100 peak  7891 weight  0.11000E+01 volume  0.29964E+03 ppm1    9 072 ppm2    1 068
ASSI { 7901}
 (( segid "BrD " and resid 73   and name HN  ))
 (  segid "BrD " and resid 73   and name HD1%)
  3 300    2 700    2 200 peak  7901 weight  0 11000E+01 volume  0 15507E+03 ppm1    8 049 ppm2    1 540
ASSI { 7911}
 (( segid "BrD " and resid 73   and name HN  ))
 (( segid "BrD " and resid 73   and name HB1 ))
  2 800    2 000    2 000 peak  7911 weight  0 11000E+01 volume  0 38621E+03 ppm1    8 045 ppm2    2 590
ASSI { 7921}
 (( segid "BrD " and resid 56   and name HN  ))
 (  segid "BrD " and resid 56   and name HD2%)
  3 100    2 400    2 400 peak  7921 weight  0 11000E+01 volume  0 19974E+03 ppm1    9.679 ppm2    1 235
ASSI { 7931}
 (( segid "BrD " and resid 22   and name HN  ))
 (  segid "BrD " and resid 22   and name HD2%)
  3 000    2 200    2 200 peak  7931 weight  0 11000E+01 volume  0 25836E+03 ppm1    9 455 ppm2    1 584
ASSI { 7941}
 (( segid "BrD " and resid 110  and name HN  ))
 (( segid "BrD " and resid 110  and name HG11))
  2 900    2 100    2 100 peak  7941 weight  0 11000E+01 volume  0 31947E+03 ppm1    8 715 ppm2    1 745
ASSI { 7951}
 (( segid "BrD " and resid 29   and name HN  ))
 (( segid "BrD " and resid 29   and name HG1 ))
  3 100    2 400    2 400 peak  7951 weight  0 11000E+01 volume  0 23530E+03 ppm1    9.152 ppm2    3 021
ASSI { 7961}
 (( segid "BrD " and resid 23   and name HN  ))
 (( segid "BrD " and resid 23   and name HB2 ))
  2.400    1 400    1 400 peak  7961 weight  0 11000E+01 volume  0 91388E+03 ppm1    9 120 ppm2    2 851
ASSI { 7971}
 (( segid "BrD " and resid 80   and name HN  ))
 (( segid "BrD " and resid 80   and name HD2 ))
  4 400    4 400    1 100 peak  7971 weight  0 11000E+01 volume  0 24560E+02 ppm1    8 007 ppm2    3 932
ASSI { 7981}
 (( segid "BrD " and resid 100  and name HN  ))
 (( segid "BrD " and resid 100  and name HB1 ))
  2 800    2.000    2 000 peak  7981 weight  0.11000E+01 volume  0 39419E+03 ppm1    8 669 ppm2    3 493
ASSI { 7991}
 (( segid "BrD " and resid 19   and name HN  ))
 (( segid "BrD " and resid 19   and name HB2 ))
  3 000    2.200    2 200 peak  7991 weight  0.11000E+01 volume  0 28394E+03 ppm1    9 187 ppm2    1 971
ASSI { 8001}
 (( segid "BrD " and resid 97   and name HN  ))
 (( segid "BrD " and resid 97   and name HG1 ))
  2 500    1 600    1 600 peak  8001 weight  0.11000E+01 volume  0.82725E+03 ppm1    8 674 ppm2    2 415
ASSI { 8011}
 (( segid "BrD " and resid 105  and name HN  ))
 (( segid "BrD " and resid 105  and name HB3 ))
  3.100    2.400    2 400 peak  8011 weight  0 11000E+01 volume  0 23309E+03 ppm1    8 487 ppm2    3 654
ASSI { 8021}
 (( segid "BrD " and resid 12   and name HN  ))
 (( segid "BrD " and resid 12   and name HB2 ))
  3 100    2 400    2 400 peak  8021 weight  0 11000E+01 volume  0 23285E+03 ppm1    9 021 ppm2    3 337
ASSI { 8031}
 (( segid "BrD " and resid 10   and name HN  ))
 (( segid "BrD " and resid 10   and name HB2 ))
  3 000    2 200    2 200 peak  8031 weight  0 11000E+01 volume  0 26676E+03 ppm1    8 886 ppm2    3 299
ASSI { 8041}
 (( segid "BrD " and resid 114  and name HN  ))
 (( segid "BrD " and resid 114  and name HA2 ))
  2.800    2 000    2 000 peak  8041 weight  0 11000E+01 volume  0 43718E+03 ppm1    8 375 ppm2    4 531
ASSI { 8051}
 (( segid "BrD " and resid 85   and name HN  ))
 (( segid "BrD " and resid 85   and name HB2 ))
  3 100    2.400    2 400 peak  8051 weight  0 11000E+01 volume  0 21741E+03 ppm1    7 517 ppm2    3 603
ASSI { 8101}
 (( segid "BrD " and resid 39   and name HN  ))
 (( segid "BrD " and resid 39   and name HB1 ))
  2 800    2 000    2 000 peak  8101 weight  0.11000E+01 volume  0 36178E+03 ppm1    9 651 ppm2    2 480
ASSI { 8111}
 (( segid "BrD " and resid 39   and name HN  ))
 (( segid "BrD " and resid 39   and name HD1 ))
  2 500    1 600    1.600 peak  8111 weight  0.11000E+01 volume  0 74538E+03 ppm1    9 653 ppm2    2 280
ASSI { 8121}
 (( segid "BrD " and resid 39   and name HN  ))
 (( segid "BrD " and resid 39   and name HG1 ))
  3 100    2 400    2.400 peak  8121 weight  0.11000E+01 volume  0 20991E+03 ppm1    9 651 ppm2    2.042
ASSI { 8131}
 (( segid "BrD " and resid 57   and name HN  ))
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  (( segid "BrD " and resid 59   and name HN  ))
     3.700     3.400      1 800 peak  8131 weight  0 11000E+01 volume  0 75880E+02 ppm1     9 355 ppm2     8 478
ASSI { 8171}
  (( segid "BrD " and resid 57   and name HN  ))
  (( segid "BrD " and resid 56   and name HB1 ))
     2 800     2 000      2 000 peak  8171 weight  0.11000E+01 volume  0 40297E+03 ppm1     9 359 ppm2     2 702
ASSI { 8191}
  (( segid "BrD " and resid 57   and name HN  ))
  (  segid "BrD " and resid 56   and name HD1%)
     3 700     3 400      1 800 peak  8191 weight  0 11000E+01 volume  0 68904E+02 ppm1     9 358 ppm2     1 547
ASSI { 8201}
  (( segid "BrD " and resid 57   and name HN  ))
  (( segid "BrD " and resid 57   and name HG2 ))
     3 700     3 400      1 800 peak  8201 weight  0 11000E+01 volume  0 72644E+02 ppm1     9 361 ppm2     2 011
ASSI { 8241}
  (( segid "BrD " and resid 28   and name HN  ))
  (( segid "BrD " and resid 24   and name HA  ))
     3.600     3 200      1 900 peak  8241 weight  0 11000E+01 volume  0 82533E+02 ppm1     8 166 ppm2     4 803
ASSI { 8251}
  (( segid "BrD " and resid 28   and name HN  ))
  (( segid "BrD " and resid 28   and name HD2 ))
     3 800     3 600      1 700 peak  8251 weight  0 11000E+01 volume  0.64220E+02 ppm1     8 166 ppm2     5 585
ASSI { 8351}
  (( segid "BrD " and resid 51   and name HN  ))
  (  segid "BrD " and resid 50   and name HG2%)
     3 000     2 200      2 200 peak  8351 weight  0 11000E+01 volume  0 27507E+03 ppm1     8 379 ppm2     0.982
ASSI { 8431}
  (( segid "BrD " and resid 117  and name HN  ))
  (  segid "BrD " and resid 116  and name HG2%)
     3 700     3 400      1 800 peak  8431 weight  0 11000E+01 volume  0 73143E+02 ppm1     8 877 ppm2     1 422
ASSI { 8471}
  (( segid "BrD " and resid 102  and name HN  ))
  (( segid "BrD " and resid 101  and name HB  ))
     3 000     2 200      2 200 peak  8471 weight  0 11000E+01 volume  0 25477E+03 ppm1     9 156 ppm2     2 531
ASSI { 8491}
  (( segid "BrD " and resid 102  and name HN  ))
  (  segid "BrD " and resid 101  and name HG2%)
     3 300     2 700      2 200 peak  8491 weight  0.11000E+01 volume  0 14766E+03 ppm1     9 156 ppm2     1 598
ASSI { 8541}
  (( segid "BrD " and resid 46   and name HN  ))
  (  segid "BrD " and resid 46   and name HD% )
     3 500     3 100      2 000 peak  8541 weight  0 11000E+01 volume  0 10722E+03 ppm1     8 562 ppm2     5 719
ASSI { 8591}
  (( segid "BrD " and resid 43   and name HN  ))
  (( segid "BrD " and resid 41   and name HA  ))
     3 000     2 200      2 200 peak  8591 weight  0 11000E+01 volume  0 24489E+03 ppm1     8 001 ppm2     4 645
ASSI { 8671}
  (( segid "BrD " and resid 111  and name HN  ))
  (( segid "BrD " and resid 110  and name HG11))
     3 600     3 200      1 900 peak  8671 weight  0 11000E+01 volume  0 81338E+02 ppm1     8 168 ppm2     1 747
ASSI { 8701}
  (( segid "BrD " and resid 111  and name HN  ))
  (  segid "BrD " and resid 110  and name HD1%)
     4 000     4.000      1 500 peak  8701 weight  0 11000E+01 volume  0 48240E+02 ppm1     8 168 ppm2     1 148
ASSI { 8731}
  (( segid "BrD " and resid 58   and name HN  ))
  (( segid "BrD " and resid 57   and name HB1 ))
     3 100     2 400      2 400 peak  8731 weight  0 11000E+01 volume  0 22478E+03 ppm1    10 051 ppm2     2 937
ASSI { 8741}
  (( segid "BrD " and resid 58   and name HN  ))
  (( segid "BrD " and resid 57   and name HB2 ))
     3 100     2 400      2 400 peak  8741 weight  0 11000E+01 volume  0 21458E+03 ppm1    10 051 ppm2     2 831
ASSI { 8761}
  (( segid "BrD " and resid 58   and name HN  ))
  (( segid "BrD " and resid 57   and name HD1 ))
     4 300     4 300      1 200 peak  8761 weight  0 11000E+01 volume  0.29553E+02 ppm1    10 051 ppm2     2 400
ASSI { 8771}
  (( segid "BrD " and resid 58   and name HN  ))
  (( segid "BrD " and resid 57   and name HD2 ))
     3 800     3 600      1 700 peak  8771 weight  0 11000E+01 volume  0 60769E+02 ppm1    10 051 ppm2     2 303
ASSI { 8781}
  (( segid "BrD " and resid 58   and name HN  ))
  (( segid "BrD " and resid 57   and name HG1 ))
     3 800     3.600      1 700 peak  8781 weight  0 11000E+01 volume  0 60094E+02 ppm1    10 051 ppm2     2 090
ASSI { 8791}
  (( segid "BrD " and resid 58   and name HN  ))
  (( segid "BrD " and resid 57   and name HG2 ))
     3 800     3 600      1 700 peak  8791 weight  0.11000E+01 volume  0 67776E+02 ppm1    10 051 ppm2     2 010
ASSI { 8821}
  (( segid "BrD " and resid 10   and name HN  ))
  (( segid "BrD " and resid 9    and name HG1 ))
     4 100     4 100      1 400 peak  8821 weight  0 11000E+01 volume  0 38664E+02 ppm1     8 885 ppm2     2 288
ASSI { 8831}
  (( segid "BrD " and resid 13   and name HN  ))
  (( segid "BrD " and resid 12   and name HB2 ))
     3 400     2 900      2 100 peak  8831 weight  0 11000E+01 volume  0 11575E+03 ppm1     8 803 ppm2     3.337
ASSI { 8841}
  (( segid "BrD " and resid 14   and name HN  ))
  (( segid "BrD " and resid 12   and name HN  ))
     2 600     1 700      1 700 peak  8841 weight  0.11000E+01 volume  0 58119E+03 ppm1     8 803 ppm2     9 004
ASSI { 8921}
  (( segid "BrD " and resid 112  and name HN  ))
  (( segid "BrD " and resid 111  and name HB1 ))
     2 700     1 800      1 800 peak  8921 weight  0 11000E+01 volume  0 53559E+03 ppm1     8 666 ppm2     2 473
ASSI { 8931}
  (( segid "BrD " and resid 112  and name HN  ))
  (( segid "BrD " and resid 111  and name HB2 ))
     3.100     2 400      2 400 peak  8931 weight  0 11000E+01 volume  0 20903E+03 ppm1     8 667 ppm2     2 363
ASSI { 8951}
  (( segid "BrD " and resid 112  and name HN  ))
  (( segid "BrD " and resid 111  and name HG1 ))
     3 800     3.600      1 700 peak  8951 weight  0 11000E+01 volume  0 66936E+02 ppm1     8.668 ppm2     1 997
ASSI { 9001}
  (( segid "BrD " and resid 105  and name HN  ))
  (( segid "BrD " and resid 104  and name HB1 ))
     2.600     1 700      1 700 peak  9001 weight  0.11000E+01 volume  0 67760E+03 ppm1     8 487 ppm2     2.536
ASSI { 9021}
  (( segid "BrD " and resid 105  and name HN  ))
  (( segid "BrD " and resid 104  and name HG1 ))
     4.800     4 800      0 700 peak  9021 weight  0.11000E+01 volume  0.16288E+02 ppm1     8 485 ppm2     2.099
ASSI { 9081}
  (( segid "BrD " and resid 109  and name HN  ))
  (( segid "BrD " and resid 108  and name HB1 ))
     2 500     1 600      1 600 peak  9081 weight  0 11000E+01 volume  0 75253E+03 ppm1     8 573 ppm2     4 614
ASSI { 9141}
  (( segid "BrD " and resid 106  and name HN  ))
  (  segid "BrD " and resid 106  and name HD% )
     3 700     3 400      1 800 peak  9141 weight  0 11000E+01 volume  0 76595E+02 ppm1     9 740 ppm2     7.511
ASSI { 9151}
  (( segid "BrD " and resid 106  and name HN  ))
  (( segid "BrD " and resid 102  and name HA  ))
     3.700     3 400      1 800 peak  9151 weight  0 11000E+01 volume  0 78592E+02 ppm1     9 740 ppm2     4 277
ASSI { 9301}
  (( segid "BrD " and resid 63   and name HN  ))
  (( segid "BrD " and resid 60   and name HA  ))
     3 800     3 600      1 700 peak  9301 weight  0 11000E+01 volume  0 67510E+02 ppm1     9.471 ppm2     4 809
ASSI { 9321}
  (( segid "BrD " and resid 63   and name HN  ))
  (( segid "BrD " and resid 62   and name HB1 ))
     2 200     1 200      1 200 peak  9321 weight  0.11000E+01 volume  0 14701E+04 ppm1     9 472 ppm2     2 654
ASSI { 9331}
  (( segid "BrD " and resid 63   and name HN  ))
  (( segid "BrD " and resid 61   and name HN  ))
     3 500     3.100      2 000 peak  9331 weight  0 11000E+01 volume  0 10977E+03 ppm1     9.475 ppm2     8 757
ASSI { 9351}
  (( segid "BrD " and resid 22   and name HN  ))
  (( segid "BrD " and resid 20   and name HA  ))
     4 100     4 100      1 400 peak  9351 weight  0.11000E+01 volume  0 39214E+02 ppm1     9 458 ppm2     4 872
ASSI { 9361}
  (( segid "BrD " and resid 22   and name HN  ))
  (( segid "BrD " and resid 19   and name HA  ))
     3 600     3 200      1 900 peak  9361 weight  0.11000E+01 volume  0 85958E+02 ppm1     9 457 ppm2     4 286
ASSI { 9391}
  (( segid "BrD " and resid 22   and name HN  ))
  (( segid "BrD " and resid 21   and name HB  ))
     2 700     1 800      1 800 peak  9391 weight  0 11000E+01 volume  0 51430E+03 ppm1     9 457 ppm2     2 491
ASSI { 9551}
  (( segid "BrD " and resid 103  and name HN  ))
  (( segid "BrD " and resid 99   and name HA  ))
     4 600     4 600      0 900 peak  9551 weight  0 11000E+01 volume  0 21373E+02 ppm1     8 695 ppm2     4 441
ASSI { 9571}
  (( segid "BrD " and resid 103  and name HN  ))
  (( segid "BrD " and resid 102  and name HG  ))
     3 200     2 600      2 300 peak  9571 weight  0 11000E+01 volume  0 17364E+03 ppm1     8 695 ppm2     2 187
ASSI { 9581}
  (( segid "BrD " and resid 103  and name HN  ))
  (  segid "BrD " and resid 101  and name HG2%)
     3 000     2.200      2 200 peak  9581 weight  0 11000E+01 volume  0 23656E+03 ppm1     8 695 ppm2     1 624
ASSI { 9591}
  (( segid "BrD " and resid 103  and name HN  ))
  (  segid "BrD " and resid 102  and name HD1%)
     3.600     3 200      1 900 peak  9591 weight  0 11000E+01 volume  0 85679E+02 ppm1     8 695 ppm2     1 308
ASSI { 9601}
  (( segid "BrD " and resid 103  and name HN  ))
  (( segid "BrD " and resid 102  and name HB2 ))
     3.200     2 600      2 300 peak  9601 weight  0 11000E+01 volume  0 18049E+03 ppm1     8 695 ppm2     1 806
ASSI { 9691}
  (( segid "BrD " and resid 18   and name HN  ))
  (( segid "BrD " and resid 18   and name HB2 ))
     2.800     2.000      2 000 peak  9691 weight  0 11000E+01 volume  0.37426E+03 ppm1     9.073 ppm2     0.909
ASSI { 9701}
  (( segid "BrD " and resid 64   and name HN  ))
  (( segid "BrD " and resid 61   and name HA  ))
     3.100     2 400      2 400 peak  9701 weight  0 11000E+01 volume  0 22483E+03 ppm1     8 584 ppm2     4 652
ASSI { 9711}
  (( segid "BrD " and resid 64   and name HN  ))
  (( segid "BrD " and resid 62   and name HA  ))
     3 900     3.800      1 600 peak  9711 weight  0 11000E+01 volume  0.56508E+02 ppm1     8.583 ppm2     4.488
ASSI { 9741}
  (( segid "BrD " and resid 64   and name HN  ))
  (( segid "BrD " and resid 63   and name HB1 ))
     2 600     1 700      1 700 peak  9741 weight  0.11000E+01 volume  0 57592E+03 ppm1     8 585 ppm2     2 902
ASSI { 9931}
  (( segid "BrD " and resid 62   and name HN  ))
  (( segid "BrD " and resid 62   and name HB2 ))
     2 900     2.100      2 100 peak  9931 weight  0.11000E+01 volume  0 30063E+03 ppm1     8 998 ppm2     1 683
ASSI { 9941}
  (( segid "BrD " and resid 62   and name HN  ))
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  (( segid "BrD " and resid 62   and name HG2 ))
     3.700     3.400     1.800 peak  9941 weight  0.11000E+01 volume  0 71463E+02 ppm1      8 998 ppm2      1 484
ASSI { 9961}
  (( segid "BrD " and resid 12   and name HN  ))
  (( segid "BrD " and resid 11   and name HD1 ))
     2 800     2 000     2 000 peak  9961 weight  0 11000E+01 volume  0 35721E+03 ppm1      9.021 ppm2      4 473
ASSI {10011}
  (( segid "BrD " and resid 25   and name HN  ))
  (( segid "BrD " and resid 22   and name HA  ))
     3 300     2 700     2 200 peak 10011 weight  0 11000E+01 volume  0 14084E+03 ppm1      9.133 ppm2      4 697
ASSI {10041}
  (( segid "BrD " and resid 24   and name HN  ))
  (( segid "BrD " and resid 23   and name HB1 ))
     2.600     1 700     1 700 peak 10041 weight  0.11000E+01 volume  0 58902E+03 ppm1      8 655 ppm2      2 934
ASSI {10051}
  (( segid "BrD " and resid 24   and name HN  ))
  (  segid "BrD " and resid 21   and name HG2%)
     3 600     3 200     1 900 peak 10051 weight  0 11000E+01 volume  0 85488E+02 ppm1      8 656 ppm2      1 610
ASSI {10071}
  (( segid "BrD " and resid 24   and name HN  ))
  (( segid "BrD " and resid 20   and name HA  ))
     3 800     3 600     1 700 peak 10071 weight  0 11000E+01 volume  0 60003E+02 ppm1      8 659 ppm2      4 888
ASSI {10101}
  (( segid "BrD " and resid 15   and name HN  ))
  (( segid "BrD " and resid 13   and name HB1 ))
     3 500     3.100     2 000 peak 10101 weight  0 11000E+01 volume  0 10487E+03 ppm1      8 599 ppm2      2 755
ASSI {10161}
  (( segid "BrD " and resid 16   and name HN  ))
  (( segid "BrD " and resid 15   and name HA  ))
     2 800     2 000     2 000 peak 10161 weight  0 11000E+01 volume  0 35770E+03 ppm1      8.796 ppm2      4 637
ASSI {10171}
  (( segid "BrD " and resid 16   and name HN  ))
  (  segid "BrD " and resid 15   and name HD% )
     3 500     3 100     2 000 peak 10171 weight  0 11000E+01 volume  0 11249E+03 ppm1      8 792 ppm2      7 660
ASSI {10211}
  (( segid "BrD " and resid 75   and name HN  ))
  (( segid "BrD " and resid 73   and name HA  ))
     3 900     3 800     1 600 peak 10211 weight  0 11000E+01 volume  0 50909E+02 ppm1      9 106 ppm2      4.820
ASSI {10271}
  (( segid "BrD " and resid 75   and name HN  ))
  (  segid "BrD " and resid 74   and name HD% )
     3 200     2.600     2.300 peak 10271 weight  0 11000E+01 volume  0 18529E+03 ppm1      9 107 ppm2      7 007
ASSI {10321}
  (( segid "BrD " and resid 96   and name HN  ))
  (( segid "BrD " and resid 95   and name HB2 ))
     2 600     1 700     1.700 peak 10321 weight  0 11000E+01 volume  0 63650E+03 ppm1      7 979 ppm2      3 345
ASSI {10341}
  (( segid "BrD " and resid 95   and name HN  ))
  (( segid "BrD " and resid 92   and name HA  ))
     3 400     2 900     2 100 peak 10341 weight  0 11000E+01 volume  0 12625E+03 ppm1      8 669 ppm2      4 792
ASSI {10361}
  (( segid "BrD " and resid 95   and name HN  ))
  (  segid "BrD " and resid 95   and name HD% )
     3 400     2.900     2 100 peak 10361 weight  0 11000E+01 volume  0 13077E+03 ppm1      8 670 ppm2      7 500
ASSI {10371}
  (( segid "BrD " and resid 96   and name HN  ))
  (  segid "BrD " and resid 96   and name HD% )
     3 300     2 700     2 200 peak 10371 weight  0 11000E+01 volume  0 14891E+03 ppm1      7 979 ppm2      7 701
ASSI {10481}
  (( segid "BrD " and resid 78   and name HN  ))
  (( segid "BrD " and resid 75   and name HA  ))
     3.100     2 400     2 400 peak 10481 weight  0 11000E+01 volume  0 20590E+03 ppm1      7.996 ppm2      4 532
ASSI {10491}
  (( segid "BrD " and resid 78   and name HN  ))
  (( segid "BrD " and resid 74   and name HA  ))
     2 800     2 000     2 000 peak 10491 weight  0 11000E+01 volume  0 36339E+03 ppm1      7 996 ppm2      4 370
ASSI {10511}
  (( segid "BrD " and resid 54   and name HN  ))
  (( segid "BrD " and resid 53   and name HB1 ))
     2 800     2.000     2 000 peak 10511 weight  0 11000E+01 volume  0 43885E+03 ppm1      9.037 ppm2      2 816
ASSI {10521}
  (( segid "BrD " and resid 54   and name HN  ))
  (  segid "BrD " and resid 50   and name HG2%)
     3 400     2 900     2 100 peak 10521 weight  0 11000E+01 volume  0 12606E+03 ppm1      9 036 ppm2      0 987
ASSI {10671}
  (( segid "BrD " and resid 82   and name HN  ))
  (( segid "BrD " and resid 78   and name HA  ))
     3 900     3.800     1.600 peak 10671 weight  0 11000E+01 volume  0 53978E+02 ppm1      6 981 ppm2      4 005
ASSI {10691}
  (( segid "BrD " and resid 81   and name HN  ))
  (( segid "BrD " and resid 80   and name HG1 ))
     3 600     3 200     1.900 peak 10691 weight  0 11000E+01 volume  0 91821E+02 ppm1      7 640 ppm2      2 349
ASSI {10701}
  (( segid "BrD " and resid 81   and name HN  ))
  (( segid "BrD " and resid 80   and name HB1 ))
     3 700     3 400     1.800 peak 10701 weight  0.11000E+01 volume  0.72987E+02 ppm1      7 640 ppm2      2.580
ASSI {10711}
  (( segid "BrD " and resid 81   and name HN  ))
  (( segid "BrD " and resid 80   and name HB2 ))
     3.700     3 400     1 800 peak 10711 weight  0 11000E+01 volume  0 72825E+02 ppm1      7 640 ppm2      2 493
ASSI {10731}
  (( segid "BrD " and resid 81   and name HN  ))
  (( segid "BrD " and resid 79   and name HA  ))
     3.900     3 800     1 600 peak 10731 weight  0 11000E+01 volume  0 55498E+02 ppm1      7 640 ppm2      4 412
ASSI {10791}
  (( segid "BrD " and resid 80   and name HN  ))
  (  segid "BrD " and resid 78   and name HD2%)
     5.500     5 500     0 000 peak 10791 weight  0.11000E+01 volume  0 63252E+00 ppm1      8 014 ppm2      0 668
ASSI {10801}
  (( segid "BrD " and resid 80   and name HN  ))
  (  segid "BrD " and resid 78   and name HD1%)
     4 400     4 400     1 100 peak 10801 weight  0 11000E+01 volume  0 27938E+02 ppm1      8.014 ppm2      0 791
ASSI {10831}
  (( segid "BrD " and resid 79   and name HN  ))
  (( segid "BrD " and resid 78   and name HB1 ))
     3.300     2 700     2 200 peak 10831 weight  0 11000E+01 volume  0 14525E+03 ppm1      8 680 ppm2      1 364
ASSI {10911}
  (( segid "BrD " and resid 86   and name HN  ))
  (( segid "BrD " and resid 83   and name HA  ))
     3 300     2 700     2 200 peak 10911 weight  0 11000E+01 volume  0 16077E+03 ppm1      8 423 ppm2      4.445
ASSI {10951}
  (( segid "BrD " and resid 87   and name HN  ))
  (( segid "BrD " and resid 86   and name HD1 ))
     3 500     3 100     2 000 peak 10951 weight  0 11000E+01 volume  0 10535E+03 ppm1      8 571 ppm2      1 898
ASSI {10961}
  (( segid "BrD " and resid 86   and name HN  ))
  (( segid "BrD " and resid 87   and name HN  ))
     3.100     2 400     2 400 peak 10961 weight  0 11000E+01 volume  0 19900E+03 ppm1      8 424 ppm2      8 553
ASSI {10971}
  (( segid "BrD " and resid 87   and name HN  ))
  (( segid "BrD " and resid 83   and name HA  ))
     4 200     4 200     1 300 peak 10971 weight  0 11000E+01 volume  0 36593E+02 ppm1      8 572 ppm2      4 445
ASSI {11061}
  (( segid "BrD " and resid 89   and name HN  ))
  (  segid "BrD " and resid 88   and name HD% )
     3 200     2 600     2 300 peak 11061 weight  0 11000E+01 volume  0 19134E+03 ppm1      8 858 ppm2      7 596
ASSI {11071}
  (( segid "BrD " and resid 89   and name HN  ))
  (( segid "BrD " and resid 91   and name HD1 ))
     5.300     5.300     0 200 peak 11071 weight  0 11000E+01 volume  0 89575E+01 ppm1      8 858 ppm2      4 559
ASSI {11081}
  (( segid "BrD " and resid 89   and name HN  ))
  (( segid "BrD " and resid 91   and name HD2 ))
     3.800     3.600     1 700 peak 11081 weight  0 11000E+01 volume  0 66703E+02 ppm1      8 858 ppm2      4 400
ASSI {11101}
  (( segid "BrD " and resid 89   and name HN  ))
  (( segid "BrD " and resid 87   and name HB1 ))
     3.800     3.600     1 700 peak 11101 weight  0 11000E+01 volume  0 67773E+02 ppm1      8 858 ppm2      2 779
ASSI {11111}
  (( segid "BrD " and resid 89   and name HN  ))
  (( segid "BrD " and resid 87   and name HB2 ))
     4.200     4 200     1 300 peak 11111 weight  0 11000E+01 volume  0 36189E+02 ppm1      8.865 ppm2      2 610
ASSI {11121}
  (( segid "BrD " and resid 92   and name HN  ))
  (( segid "BrD " and resid 91   and name HB1 ))
     3 200     2.600     2 300 peak 11121 weight  0 11000E+01 volume  0 16770E+03 ppm1      8 876 ppm2      3 059
ASSI {11221}
  (( segid "BrD " and resid 30   and name HN  ))
  (( segid "BrD " and resid 28   and name HN  ))
     4 100     4 100     1 400 peak 11221 weight  0 11000E+01 volume  0.38088E+02 ppm1     12 275 ppm2      8 143
ASSI {11261}
  (( segid "BrD " and resid 31   and name HN  ))
  (( segid "BrD " and resid 29   and name HG1 ))
     5.100     5.100     0 400 peak 11261 weight  0 11000E+01 volume  0 11011E+02 ppm1      8 486 ppm2      2 997
ASSI {11311}
  (( segid "BrD " and resid 31   and name HN  ))
  (  segid "BrD " and resid 102  and name HD1%)
     3 300     2 700     2 200 peak 11311 weight  0.11000E+01 volume  0 14151E+03 ppm1      8 480 ppm2      1 314
ASSI {11331}
  (( segid "BrD " and resid 32   and name HN  ))
  (( segid "BrD " and resid 33   and name HD1 ))
     3.900     3 800     1 600 peak 11331 weight  0 11000E+01 volume  0 57286E+02 ppm1      7.738 ppm2      2 782
ASSI {11341}
  (( segid "BrD " and resid 32   and name HN  ))
  (( segid "BrD " and resid 33   and name HD2 ))
     2.500     1 600     1 600 peak 11341 weight  0.11000E+01 volume  0 82617E+03 ppm1      7 739 ppm2      2 174
ASSI {11381}
  (( segid "BrD " and resid 34   and name HN  ))
  (( segid "BrD " and resid 32   and name HA  ))
     4.200     4 200     1.300 peak 11381 weight  0.11000E+01 volume  0 36612E+02 ppm1      8 183 ppm2      4 975
ASSI {11411}
  (( segid "BrD " and resid 34   and name HN  ))
  (( segid "BrD " and resid 33   and name HD1 ))
     2 600     1 700     1 700 peak 11411 weight  0 11000E+01 volume  0.60528E+03 ppm1      8 181 ppm2      2 784
ASSI {11421}
  (( segid "BrD " and resid 34   and name HN  ))
  (( segid "BrD " and resid 33   and name HD2 ))
     3.300     2 700     2 200 peak 11421 weight  0.11000E+01 volume  0.15559E+03 ppm1      8 184 ppm2      2.174
ASSI {11461}
  (( segid "BrD " and resid 34   and name HN  ))
  (( segid "BrD " and resid 33   and name HB1 ))
     3.500     3.100     2 000 peak 11461 weight  0.11000E+01 volume  0 11065E+03 ppm1      8.178 ppm2      1 094
ASSI {11471}
  (( segid "BrD " and resid 34   and name HN  ))
  (( segid "BrD " and resid 33   and name HG1 ))
     4 100     4.100     1 400 peak 11471 weight  0 11000E+01 volume  0 41672E+02 ppm1      8 177 ppm2      0 840
ASSI {11481}
  (( segid "BrD " and resid 34   and name HN  ))
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(( segid "BrD " and resid 33   and name HA  ))
   3 200     2.600     2 300 peak 11481 weight  0 11000E+01 volume  0 17351E+03 ppm1     8 182 ppm2     4 363
ASSI {11501}
  (( segid "BrD " and resid 36   and name HN  ))
  (( segid "BrD " and resid 35   and name HB1 ))
   4 000     4 000     1 500 peak 11501 weight  0 11000E+01 volume  0 43329E+02 ppm1     8 308 ppm2     2 840
ASSI {11611}
  (( segid "BrD " and resid 67   and name HN  ))
  (( segid "BrD " and resid 65   and name HB2 ))
   3.800     3.600     1 700 peak 11611 weight  0 11000E+01 volume  0 63235E+02 ppm1     8 832 ppm2     3 380
ASSI {11621}
  (( segid "BrD " and resid 67   and name HN  ))
  (( segid "BrD " and resid 66   and name HG1 ))
   3 700     3 400     1 800 peak 11621 weight  0 11000E+01 volume  0 76792E+02 ppm1     8.832 ppm2     2 146
ASSI {11641}
  (( segid "BrD " and resid 68   and name HN  ))
  (( segid "BrD " and resid 66   and name HA  ))
   2 500     1.600     1 600 peak 11641 weight  0 11000E+01 volume  0 80687E+03 ppm1     8 626 ppm2     5 012
ASSI {11681}
  (( segid "BrD " and resid 68   and name HN  ))
  (  segid "BrD " and resid 69   and name HG2%)
   3 400     2 900     2 100 peak 11681 weight  0 11000E+01 volume  0 13257E+03 ppm1     8 626 ppm2     1 437
ASSI {11691}
  (( segid "BrD " and resid 68   and name HN  ))
  (  segid "BrD " and resid 69   and name HG1%)
   3 700     3 400     1 800 peak 11691 weight  0 11000E+01 volume  0 73874E+02 ppm1     8 626 ppm2     1 562
ASSI {11721}
  (( segid "BrD " and resid 69   and name HN  ))
  (  segid "BrD " and resid 68   and name HD% )
   3 500     3.100     2 000 peak 11721 weight  0 11000E+01 volume  0 11106E+03 ppm1     8 306 ppm2     7 782
ASSI {11781}
  (( segid "BrD " and resid 70   and name HN  ))
  (( segid "BrD " and resid 68   and name HA  ))
   3 200     2 600     2 300 peak 11781 weight  0 11000E+01 volume  0 19118E+03 ppm1     8 039 ppm2     5 135
ASSI {11791}
  (( segid "BrD " and resid 74   and name HN  ))
  (  segid "BrD " and resid 73   and name HD2%)
   4.400     4 400     1 100 peak 11791 weight  0 11000E+01 volume  0 24720E+02 ppm1     7 536 ppm2     1 502
ASSI {11801}
  (( segid "BrD " and resid 74   and name HN  ))
  (  segid "BrD " and resid 73   and name HD1%)
   4 100     4 100     1 400 peak 11801 weight  0 11000E+01 volume  0 39673E+02 ppm1     7 536 ppm2     1.531
ASSI {11811}
  (( segid "BrD " and resid 74   and name HN  ))
  (( segid "BrD " and resid 73   and name HG  ))
   3 100     2.400     2 400 peak 11811 weight  0 11000E+01 volume  0 21474E+03 ppm1     7 537 ppm2     2 401
ASSI {11821}
  (( segid "BrD " and resid 74   and name HN  ))
  (( segid "BrD " and resid 73   and name HB2 ))
   2 900     2 100     2 100 peak 11821 weight  0 11000E+01 volume  0 29959E+03 ppm1     7 536 ppm2     2 498
ASSI {11831}
  (( segid "BrD " and resid 74   and name HN  ))
  (( segid "BrD " and resid 73   and name HB1 ))
   3 000     2 200     2 200 peak 11831 weight  0 11000E+01 volume  0 27375E+03 ppm1     7 537 ppm2     2.603
ASSI {11871}
  (( segid "BrD " and resid 73   and name HN  ))
  (  segid "BrD " and resid 76   and name HB% )
   3 300     2.700     2 200 peak 11871 weight  0.11000E+01 volume  0 13672E+03 ppm1     8 046 ppm2     2 116
ASSI {11901}
  (( segid "BrD " and resid 74   and name HN  ))
  (  segid "BrD " and resid 18   and name HD1%)
   3 700     3 400     1 800 peak 11901 weight  0 11000E+01 volume  0 74433E+02 ppm1     7 536 ppm2     1.076
ASSI {11981}
  (( segid "BrD " and resid 98   and name HN  ))
  (( segid "BrD " and resid 97   and name HB1 ))
   2 500     1 600     1 600 peak 11981 weight  0 11000E+01 volume  0 78973E+03 ppm1     9 125 ppm2     2.698
ASSI {11991}
  (( segid "BrD " and resid 98   and name HN  ))
  (( segid "BrD " and resid 97   and name HG1 ))
   3 100     2 400     2 400 peak 11991 weight  0 11000E+01 volume  0 20137E+03 ppm1     9 125 ppm2     2 426
ASSI {12001}
  (( segid "BrD " and resid 98   and name HN  ))
  (( segid "BrD " and resid 97   and name HG2 ))
   3 100     2 400     2 400 peak 12001 weight  0 11000E+01 volume  0 20070E+03 ppm1     9 124 ppm2     2 189
ASSI {12171}
  (( segid "BrD " and resid 101  and name HN  ))
  (( segid "BrD " and resid 99   and name HA  ))
   4 000     4 000     1 500 peak 12171 weight  0 11000E+01 volume  0.46069E+02 ppm1     8.513 ppm2     4 447
ASSI {12181}
  (( segid "BrD " and resid 101  and name HN  ))
  (( segid "BrD " and resid 97   and name HA  ))
   3 100     2 400     2 400 peak 12181 weight  0 11000E+01 volume  0 20943E+03 ppm1     8 513 ppm2     4 811
ASSI {12191}
  (( segid "BrD " and resid 103  and name HN  ))
  (( segid "BrD " and resid 102  and name HB1 ))
   2.800     2.000     2.000 peak 12191 weight  0 11000E+01 volume  0 37773E+03 ppm1     8 696 ppm2     2 012
ASSI {12201}
  (( segid "BrD " and resid 104  and name HN  ))
  (( segid "BrD " and resid 100  and name HA  ))
   3 200     2 600     2.300 peak 12201 weight  0 11000E+01 volume  0 18477E+03 ppm1     7 763 ppm2     4 936
ASSI {12231}
  (( segid "BrD " and resid 107  and name HN  ))
  (( segid "BrD " and resid 104  and name HA  ))
   3 000     2 200     2 200 peak 12231 weight  0 11000E+01 volume  0 26295E+03 ppm1     8 981 ppm2     4 682
ASSI {12321}
  (( segid "BrD " and resid 110  and name HN  ))
  (( segid "BrD " and resid 109  and name HD1 ))
   3 500     3 100     2 000 peak 12321 weight  0 11000E+01 volume  0.10959E+03 ppm1     8 714 ppm2     2.010
ASSI {12331}
  (( segid "BrD " and resid 110  and name HN  ))
  (( segid "BrD " and resid 109  and name HB1 ))
   2 700     1.800     1 800 peak 12331 weight  0 11000E+01 volume  0 48783E+03 ppm1     8 714 ppm2     2 337
ASSI {12341}
  (( segid "BrD " and resid 110  and name HN  ))
  (( segid "BrD " and resid 109  and name HG1 ))
   3 000     2 200     2 200 peak 12341 weight  0 11000E+01 volume  0 26294E+03 ppm1     8 714 ppm2     1 440
ASSI {12351}
  (( segid "BrD " and resid 111  and name HN  ))
  (( segid "BrD " and resid 110  and name HG12))
   3 000     2 200     2 200 peak 12351 weight  0.11000E+01 volume  0 27526E+03 ppm1     8 168 ppm2     1 680
ASSI {12361}
  (( segid "BrD " and resid 112  and name HN  ))
  (( segid "BrD " and resid 111  and name HG2 ))
   3 200     2 600     2 300 peak 12361 weight  0 11000E+01 volume  0 16739E+03 ppm1     8 668 ppm2     1 909
ASSI {12371}
  (( segid "BrD " and resid 113  and name HN  ))
  (( segid "BrD " and resid 110  and name HA  ))
   3 600     3 200     1 900 peak 12371 weight  0 11000E+01 volume  0 80563E+02 ppm1     8 217 ppm2     4 425
ASSI {12381}
  (( segid "BrD " and resid 113  and name HN  ))
  (( segid "BrD " and resid 111  and name HB1 ))
   3.900     3 800     1 600 peak 12381 weight  0 11000E+01 volume  0 57596E+02 ppm1     8 219 ppm2     2 486
ASSI {12391}
  (( segid "BrD " and resid 113  and name HN  ))
  (( segid "BrD " and resid 111  and name HB2 ))
   3 800     3 600     1 700 peak 12391 weight  0 11000E+01 volume  0.67480E+02 ppm1     8 218 ppm2     2 364
ASSI {12531}
  (( segid "BrD " and resid 48   and name HN  ))
  (( segid "BrD " and resid 47   and name HB1 ))
   4 300     4 300     1 200 peak 12531 weight  0 11000E+01 volume  0 28319E+02 ppm1     8 307 ppm2     3 796
ASSI {12541}
  (( segid "BrD " and resid 48   and name HN  ))
  (( segid "BrD " and resid 46   and name HA  ))
   4 000     4 000     1 500 peak 12541 weight  0 11000E+01 volume  0 44246E+02 ppm1     8 307 ppm2     4 152
ASSI {12551}
  (( segid "BrD " and resid 48   and name HN  ))
  (( segid "BrD " and resid 47   and name HB2 ))
   4 200     4 200     1 300 peak 12551 weight  0 11000E+01 volume  0 35395E+02 ppm1     8 307 ppm2     3 408
ASSI {12561}
  (( segid "BrD " and resid 47   and name HN  ))
  (  segid "BrD " and resid 46   and name HD% )
   3 500     3 100     2 000 peak 12561 weight  0 11000E+01 volume  0 10097E+03 ppm1     8 832 ppm2     5.727
ASSI {12571}
  (( segid "BrD " and resid 47   and name HN  ))
  (  segid "BrD " and resid 47   and name HD% )
   3 100     2 400     2.400 peak 12571 weight  0 11000E+01 volume  0 23274E+03 ppm1     8 833 ppm2     7 944
ASSI {12631}
  (( segid "BrD " and resid 51   and name HN  ))
  (( segid "BrD " and resid 50   and name HA  ))
   2 600     1 700     1 700 peak 12631 weight  0.11000E+01 volume  0 65616E+03 ppm1     8 377 ppm2     4 523
ASSI {12641}
  (( segid "BrD " and resid 52   and name HN  ))
  (( segid "BrD " and resid 51   and name HB1 ))
   3 400     2 900     2 100 peak 12641 weight  0 11000E+01 volume  0 11270E+03 ppm1     9 003 ppm2     1 995
ASSI {12651}
  (( segid "BrD " and resid 52   and name HN  ))
  (( segid "BrD " and resid 51   and name HG1 ))
   5 500     5 500     0 000 peak 12651 weight  0 11000E+01 volume  0 88686E+00 ppm1     9.003 ppm2     1 926
ASSI {12661}
  (( segid "BrD " and resid 52   and name HN  ))
  (( segid "BrD " and resid 51   and name HG2 ))
   3 400     2 900     2 100 peak 12661 weight  0 11000E+01 volume  0 11315E+03 ppm1     9 003 ppm2     1 780
ASSI {12671}
  (( segid "BrD " and resid 52   and name HN  ))
  (( segid "BrD " and resid 51   and name HB2 ))
   3.200     2 600     2.300 peak 12671 weight  0 11000E+01 volume  0 16847E+03 ppm1     9.004 ppm2     1 818
ASSI {12681}
  (( segid "BrD " and resid 52   and name HN  ))
  (  segid "BrD " and resid 50   and name HG2%)
   2 800     2.000     2 000 peak 12681 weight  0 11000E+01 volume  0.38955E+03 ppm1     9.002 ppm2     0 991
ASSI {12731}
  (( segid "BrD " and resid 42   and name HN  ))
  (( segid "BrD " and resid 41   and name HA  ))
   3.400     2 900     2 100 peak 12731 weight  0 11000E+01 volume  0 12554E+03 ppm1     7 822 ppm2     4.650
ASSI {12771}
  (( segid "BrD " and resid 42   and name HN  ))
  (  segid "BrD " and resid 41   and name HG2%)
   4 200     4 200     1.300 peak 12771 weight  0 11000E+01 volume  0 34295E+02 ppm1     7 821 ppm2     1 874
ASSI {12781}
  (( segid "BrD " and resid 97   and name HN  ))
  (  segid "BrD " and resid 96   and name HD% )
   3 300     2 700     2 200 peak 12781 weight  0.11000E+01 volume  0 13710E+03 ppm1     8 674 ppm2     7 701
ASSI {12791}
  (( segid "BrD " and resid 20   and name HN  ))
  (( segid "BrD " and resid 19   and name HG1 ))
   3 400     2 900     2 100 peak 12791 weight  0 11000E+01 volume  0 11346E+03 ppm1     8 146 ppm2     1 887
ASSI {12801}
  (( segid "BrD " and resid 19   and name HN  ))
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(( segid "BrD " and resid 18   and name HB2 ))
   3 400     2 900     2 100 peak 12801 weight  0.11000E+01 volume  0 11595E+03 ppm1       9 186 ppm2      0 901
ASSI {12811}
   (( segid "BrD " and resid 19   and name HN  ))
   (  segid "BrD " and resid 63   and name HD1%)
   3 100     2 400     2 400 peak 12811 weight  0 11000E+01 volume  0 22952E+03 ppm1       9.186 ppm2      1 642
ASSI {12821}
   (( segid "BrD " and resid 19   and name HN  ))
   (  segid "BrD " and resid 63   and name HD2%)
   3 000     2 200     2 200 peak 12821 weight  0 11000E+01 volume  0.27823E+03 ppm1       9 187 ppm2      1 476
ASSI {12831}
   (( segid "BrD " and resid 19   and name HN  ))
   (( segid "BrD " and resid 16   and name HA  ))
   3.000     2 200     2 200 peak 12831 weight  0.11000E+01 volume  0.27123E+03 ppm1       9 187 ppm2      4 516
ASSI {12871}
   (( segid "BrD " and resid 20   and name HN  ))
   (( segid "BrD " and resid 18   and name HG  ))
   3 800     3 600     1 700 peak 12871 weight  0 11000E+01 volume  0 64336E+02 ppm1       8 147 ppm2      2 290
ASSI {12931}
   (( segid "BrD " and resid 23   and name HN  ))
   (( segid "BrD " and resid 22   and name HB1 ))
   2 600     1 700     1 700 peak 12931 weight  0 11000E+01 volume  0 65708E+03 ppm1       9 120 ppm2      2 697
ASSI {12941}
   (( segid "BrD " and resid 23   and name HN  ))
   (( segid "BrD " and resid 22   and name HB2 ))
   2 800     2 000     2 000 peak 12941 weight  0 11000E+01 volume  0.39331E+03 ppm1       9 122 ppm2      2 310
ASSI {13051}
   (( segid "BrD " and resid 27   and name HN  ))
   (( segid "BrD " and resid 26   and name HD1 ))
   2 700     1 800     1 800 peak 13051 weight  0.11000E+01 volume  0 47384E+03 ppm1       8 168 ppm2      2 127
ASSI {13071}
   (( segid "BrD " and resid 27   and name HN  ))
   (( segid "BrD " and resid 24   and name HG1 ))
   3 500     3 100     2 000 peak 13071 weight  0 11000E+01 volume  0 10804E+03 ppm1       8 170 ppm2      3 447
ASSI {13081}
   (( segid "BrD " and resid 27   and name HN  ))
   (( segid "BrD " and resid 24   and name HG2 ))
   3 700     3 400     1 800 peak 13081 weight  0 11000E+01 volume  0 74378E+02 ppm1       8 170 ppm2      3 074
ASSI {13141}
   (( segid "BrD " and resid 60   and name HN  ))
   (( segid "BrD " and resid 59   and name HB2 ))
   2 900     2 100     2 100 peak 13141 weight  0 11000E+01 volume  0 32659E+03 ppm1       8 565 ppm2      2 522
ASSI {13151}
   (( segid "BrD " and resid 65   and name HN  ))
   (( segid "BrD " and resid 64   and name HG1 ))
   3 300     2 700     2 200 peak 13151 weight  0 11000E+01 volume  0 14156E+03 ppm1       8 565 ppm2      2 203
ASSI {13211}
   (( segid "BrD " and resid 15   and name HN  ))
   (( segid "BrD " and resid 14   and name HG  ))
   3 700     3 400     1 800 peak 13211 weight  0.11000E+01 volume  0 73008E+02 ppm1       8 597 ppm2      2 087
ASSI {13281}
   (( segid "BrD " and resid 65   and name HD21))
   (( segid "BrD " and resid 64   and name HB1 ))
   3 600     3 200     1 900 peak 13281 weight  0 11000E+01 volume  0 89819E+02 ppm1       8 205 ppm2      2 662
ASSI {13291}
   (( segid "BrD " and resid 65   and name HD22))
   (( segid "BrD " and resid 64   and name HB1 ))
   3 600     3 200     1 900 peak 13291 weight  0 11000E+01 volume  0.84418E+02 ppm1       7 576 ppm2      2 662
ASSI {13321}
   (( segid "BrD " and resid 93   and name HN  ))
   (( segid "BrD " and resid 93   and name HB1 ))
   4 100     4 100     1 400 peak 13321 weight  0 11000E+01 volume  0 42284E+02 ppm1       8 713 ppm2      5 009
ASSI {13331}
   (( segid "BrD " and resid 94   and name HN  ))
   (( segid "BrD " and resid 93   and name HB1 ))
   3.700     3 400     1 800 peak 13331 weight  0 11000E+01 volume  0 78957E+02 ppm1       9.679 ppm2      5 000
ASSI {13341}
   (( segid "BrD " and resid 17   and name HN  ))
   (( segid "BrD " and resid 16   and name HB1 ))
   3.400     2 900     2 100 peak 13341 weight  0.11000E+01 volume  0 11732E+03 ppm1       8 670 ppm2      4 602
ASSI {13351}
   (( segid "BrD " and resid 62   and name HN  ))
   (( segid "BrD " and resid 62   and name HD2 ))
   2 700     1.800     1 800 peak 13351 weight  0 11000E+01 volume  0 44005E+03 ppm1       8 998 ppm2      2 658
ASSI {13361}
   (( segid "BrD " and resid 86   and name HN  ))
   (( segid "BrD " and resid 86   and name HG1 ))
   4 100     4 100     1 400 peak 13361 weight  0 11000E+01 volume  0 42972E+02 ppm1       8 423 ppm2      1 920
ASSI {13371}
   (( segid "BrD " and resid 17   and name HN  ))
   (( segid "BrD " and resid 14   and name HA  ))
   2 600     1 700     1 700 peak 13371 weight  0 11000E+01 volume  0 66944E+03 ppm1       8 670 ppm2      4 652
ASSI {13381}
   (( segid "BrD " and resid 18   and name HN  ))
   (( segid "BrD " and resid 15   and name HA  ))
   3 800     3.600     1 700 peak 13381 weight  0 11000E+01 volume  0 66429E+02 ppm1       9.073 ppm2      4 620
ASSI {13391}
   (( segid "BrD " and resid 19   and name HN  ))
   (( segid "BrD " and resid 18   and name HN  ))
   2 300     1 300     1 300 peak 13391 weight  0 11000E+01 volume  0 12618E+04 ppm1       9 186 ppm2      9 067
ASSI {13401}
   (( segid "BrD " and resid 59   and name HN  ))
   (( segid "BrD " and resid 56   and name HA  ))
   3 100     2 400     2 400 peak 13401 weight  0 11000E+01 volume  0 22047E+03 ppm1       8 498 ppm2      4 643
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ASSI {13421}
   (( segid "BrD " and resid 79   and name HN  ))
   (( segid "BrD " and resid 75   and name HA  ))
   4 000     4 000     1 500 peak 13421 weight  0 11000E+01 volume  0 47743E+02 ppm1       8 680 ppm2      4 518
ASSI {13431}
   (( segid "BrD " and resid 81   and name HN  ))
   (( segid "BrD " and resid 77   and name HA  ))
   4 500     4 500     1 000 peak 13431 weight  0 11000E+01 volume  0 23511E+02 ppm1       7 639 ppm2      4 978
ASSI {13441}
   (( segid "BrD " and resid 85   and name HN  ))
   (( segid "BrD " and resid 83   and name HA  ))
   3 600     3.200     1 900 peak 13441 weight  0.11000E+01 volume  0 85635E+02 ppm1       7 519 ppm2      4 441
ASSI {13451}
   (( segid "BrD " and resid 85   and name HN  ))
   (( segid "BrD " and resid 81   and name HA  ))
   2 500     1 600     1 600 peak 13451 weight  0 11000E+01 volume  0 75325E+03 ppm1       7 517 ppm2      3 646
ASSI {13461}
   (( segid "BrD " and resid 88   and name HN  ))
   (( segid "BrD " and resid 84   and name HA  ))
   2.800     2 000     2 000 peak 13461 weight  0 11000E+01 volume  0 40309E+03 ppm1       8 357 ppm2      4 922
ASSI {13481}
   (( segid "BrD " and resid 81   and name HN  ))
   (( segid "BrD " and resid 83   and name HN  ))
   3.900     3 800     1.600 peak 13481 weight  0 11000E+01 volume  0 50469E+02 ppm1       7 640 ppm2      9 655
ASSI {13491}
   (( segid "BrD " and resid 96   and name HN  ))
   (( segid "BrD " and resid 93   and name HA  ))
   3 700     3 400     1.800 peak 13491 weight  0.11000E+01 volume  0 70852E+02 ppm1       7 981 ppm2      5 013
ASSI {13501}
   (( segid "BrD " and resid 109  and name HN  ))
   (( segid "BrD " and resid 105  and name HA  ))
   4 600     4 600     0 900 peak 13501 weight  0 11000E+01 volume  0 18885E+02 ppm1       8 574 ppm2      4 935
ASSI {13511}
   (( segid "BrD " and resid 110  and name HN  ))
   (( segid "BrD " and resid 108  and name HA  ))
   3 500     3 100     2 000 peak 13511 weight  0 11000E+01 volume  0 11166E+03 ppm1       8 714 ppm2      4 818
ASSI {13521}
   (( segid "BrD " and resid 92   and name HN  ))
   (( segid "BrD " and resid 91   and name HA  ))
   3 200     2 600     2 300 peak 13521 weight  0 11000E+01 volume  0 16456E+03 ppm1       8 873 ppm2      5 343
ASSI {13541}
   (( segid "BrD " and resid 98   and name HN  ))
   (( segid "BrD " and resid 100  and name HN  ))
   2 900     2 100     2 100 peak 13541 weight  0 11000E+01 volume  0 30894E+03 ppm1       9 125 ppm2      8 653
ASSI {13551}
   (( segid "BrD " and resid 103  and name HN  ))
   (( segid "BrD " and resid 101  and name HN  ))
   2.900     2 100     2 100 peak 13551 weight  0 11000E+01 volume  0 34725E+03 ppm1       8 696 ppm2      8 519
ASSI {13561}
   (( segid "BrD " and resid 32   and name HN  ))
   (( segid "BrD " and resid 30   and name HA  ))
   4.400     4 400     1 100 peak 13561 weight  0 11000E+61 volume  0 25941E+02 ppm1       7.739 ppm2      5 445
ASSI {13571}
   (( segid "BrD " and resid 24   and name HN  ))
   (( segid "BrD " and resid 23   and name HB2 ))
   2 800     2 000     2 000 peak 13571 weight  0 11000E+01 volume  0 42825E+03 ppm1       8 655 ppm2      2 870
ASSI {13581}
   (( segid "BrD " and resid 73   and name HN  ))
   (( segid "BrD " and resid 75   and name HN  ))
   4.000     4 000     1 500 peak 13581 weight  0 11000E+01 volume  0 46662E+02 ppm1       8 045 ppm2      9 084
ASSI {13591}
   (( segid "BrD " and resid 62   and name HN  ))
   (( segid "BrD " and resid 61   and name HG1 ))
   3 900     3 800     1 600 peak 13591 weight  0 11000E+01 volume  0 54843E+02 ppm1       8 999 ppm2      2 952
ASSI {13611}
   (( segid "BrD " and resid 67   and name HN  ))
   (( segid "BrD " and resid 65   and name HB1 ))
   2 800     2 000     2 000 peak 13611 weight  0 11000E+01 volume  0 36617E+03 ppm1       8 832 ppm2      3 626
ASSI {13621}
   (( segid "BrD " and resid 75   and name HN  ))
   (( segid "BrD " and resid 74   and name HB2 ))
   3 200     2 600     2 300 peak 13621 weight  0 11000E+01 volume  0 17250E+03 ppm1       9 106 ppm2      2 988
ASSI {13641}
   (( segid "BrD " and resid 104  and name HN  ))
   (( segid "BrD " and resid 106  and name HN  ))
   4.900     4 900     0 600 peak 13641 weight  0 11000E+01 volume  0 14134E+02 ppm1       7 763 ppm2      9.736
ASSI {13671}
   (( segid "BrD " and resid 74   and name HN  ))
   (  segid "BrD " and resid 18   and name HD2%)
   3 900     3 800     1 600 peak 13671 weight  0 11000E+01 volume  0 56031E+02 ppm1       7 545 ppm2      0.414
ASSI {13701}
   (( segid "BrD " and resid 61   and name HN  ))
   (( segid "BrD " and resid 61   and name HB1 ))
   2.800     2 000     2 000 peak 13701 weight  0 11000E+01 volume  0 41690E+03 ppm1       8 743 ppm2      2.837
ASSI {13711}
   (( segid "BrD " and resid 62   and name HN  ))
   (( segid "BrD " and resid 61   and name HB1 ))
   2 800     2 000     2 000 peak 13711 weight  0 11000E+01 volume  0 40898E+03 ppm1       8 998 ppm2      2 853
ASSI {13731}
   (( segid "BrD " and resid 25   and name HN  ))
   (( segid "BrD " and resid 21   and name HA  ))
   2 900     2 100     2 100 peak 13731 weight  0 11000E+01 volume  0 30325E+03 ppm1       9 134 ppm2      4 393
ASSI {13741}
   (( segid "BrD " and resid 63   and name HN  ))
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(( segid "BrD " and resid 59   and name HA  ))
   3.200     2.600     2.300 peak 13741 weight  0.11000E+01 volume  0.16317E+03 ppm1      9.472 ppm2      4.926
ASSI {13761}
  (( segid "BrD " and resid 74   and name HN  ))
  (( segid "BrD " and resid 71   and name HA  ))
   3 200     2 600     2 300 peak 13761 weight  0 11000E+01 volume  0.19208E+03 ppm1      7.536 ppm2      4 622
ASSI {13771}
  (( segid "BrD " and resid 75   and name HN  ))
  (( segid "BrD " and resid 71   and name HA  ))
   3 100     2 400     2 400 peak 13771 weight  0 11000E+01 volume  0.21726E+03 ppm1      9 106 ppm2      4.628
ASSI {13781}
  (( segid "BrD " and resid 77   and name HN  ))
  (( segid "BrD " and resid 74   and name HA  ))
   3 200     2 600     2 300 peak 13781 weight  0 11000E+01 volume  0 16504E+03 ppm1      7.996 ppm2      4 371
ASSI {13791}
  (( segid "BrD " and resid 105  and name HN  ))
  (( segid "BrD " and resid 101  and name HA  ))
   3 200     2 600     2 300 peak 13791 weight  0 11000E+01 volume  0 19414E+03 ppm1      8 487 ppm2      4 253
ASSI {13801}
  (( segid "BrD " and resid 26   and name HN  ))
  (( segid "BrD " and resid 24   and name HA  ))
   3 900     3 800     1 600 peak 13801 weight  0 11000E+01 volume  0.52793E+02 ppm1      9 196 ppm2      4 755
ASSI {13811}
  (( segid "BrD " and resid 26   and name HN  ))
  (( segid "BrD " and resid 25   and name HA  ))
   3 800     3 600     1 700 peak 13811 weight  0 11000E+01 volume  0.62704E+02 ppm1      9 196 ppm2      4 415
ASSI {13821}
  (( segid "BrD " and resid 29   and name HN  ))
  (( segid "BrD " and resid 25   and name HA  ))
   5 500     5 500     0 000 peak 13821 weight  0 11000E+01 volume  0.27795E-01 ppm1      9 152 ppm2      4 451
ASSI {13831}
  (( segid "BrD " and resid 54   and name HN  ))
  (( segid "BrD " and resid 55   and name HN  ))
   2 900     2 100     2 100 peak 13831 weight  0 11000E+01 volume  0 31830E+03 ppm1      9 037 ppm2      7 972
ASSI {13851}
  (( segid "BrD " and resid 48   and name HN  ))
  (  segid "BrD " and resid 47   and name HD% )
   3 900     3 800     1 600 peak 13851 weight  0 11000E+01 volume  0 57580E+02 ppm1      8 307 ppm2      7 949
ASSI {13861}
  (( segid "BrD " and resid 96   and name HN  ))
  (  segid "BrD " and resid 95   and name HD% )
   3 500     3 100     2 000 peak 13861 weight  0 11000E+01 volume  0 10869E+03 ppm1      7 979 ppm2      7 498
ASSI {14011}
  (( segid "BrD " and resid 108  and name HN  ))
  (  segid "BrD " and resid 107  and name HD% )
   4 300     4 300     1 200 peak 14011 weight  0 11000E+01 volume  0 30492E+02 ppm1      8 528 ppm2      7.782
ASSI {14881}
  (( segid "BrD " and resid 54   and name HN  ))
  (( segid "BrD " and resid 54   and name HG1 ))
   4 500     4 500     1 000 peak 14881 weight  0 11000E+01 volume  0 23500E+02 ppm1      9 038 ppm2      3.297
ASSI {15591}
  (( segid "BrD " and resid 32   and name HE1 ))
  (( segid "BrD " and resid 32   and name HB2 ))
   4 000     4 000     1 500 peak 15591 weight  0 11000E+01 volume  0 47456E+02 ppm1     11 081 ppm2      3 958
ASSI {15601}
  (( segid "BrD " and resid 32   and name HE1 ))
  (( segid "BrD " and resid 32   and name HB1 ))
   5 200     5 200     0.300 peak 15601 weight  0 11000E+01 volume  0 94290E+01 ppm1     11.081 ppm2      4 201
ASSI {  111}
  (( segid "BrD " and resid 99   and name HN  ))
  (( segid "BrD " and resid 34   and name HZ  ))
   3 100     2 400     2 400 peak   111 weight  0 10000E+01 volume  0 20460E+03 ppm1      8 936 ppm2      7 899
ASSI {  801}
  (( segid "BrD " and resid 97   and name HN  ))
  (( segid "BrD " and resid 97   and name HE1 ))
   4 000     4 000     1 500 peak   801 weight  0 10000E+01 volume  0 47904E+02 ppm1      8 673 ppm2      3 572
ASSI {  931}
  (( segid "BrD " and resid 117  and name HN  ))
  (( segid "BrD " and resid 116  and name HN  ))
   3 500     3 100     2.000 peak   931 weight  0 10000E+01 volume  0 10704E+03 ppm1      8 883 ppm2      8 075
ASSI { 1891}
  (( segid "BrD " and resid 83   and name HN  ))
  (( segid "BrD " and resid 85   and name HN  ))
   4 000     4 000     1 500 peak  1891 weight  0 10000E+01 volume  0 44105E+02 ppm1      9 660 ppm2      7 505
ASSI { 2331}
  (( segid "BrD " and resid 49   and name HN  ))
  (( segid "BrD " and resid 50   and name HA  ))
   4 000     4 000     1.500 peak  2331 weight  0 10000E+01 volume  0 49544E+02 ppm1      7 761 ppm2      4 525
ASSI { 2631}
  (( segid "BrD " and resid 103  and name HN  ))
  (  segid "BrD " and resid 82   and name HD% )
   3 800     3 600     1 700 peak  2631 weight  0 10000E+01 volume  0 64814E+02 ppm1      8 695 ppm2      7 246
ASSI { 3601}
  (( segid "BrD " and resid 9    and name HN  ))
  (( segid "BrD " and resid 9    and name HA  ))
   2 900     2 100     2 100 peak  3601 weight  0.10000E+01 volume  0 32855E+03 ppm1      9 052 ppm2      4 936
ASSI { 3751}
  (( segid "BrD " and resid 56   and name HN  ))
  (( segid "BrD " and resid 35   and name HA  ))
   3 200     2 600     2 300 peak  3751 weight  0 10000E+01 volume  0 18743E+03 ppm1      9 678 ppm2      4.895
ASSI { 4371}
  (( segid "BrD " and resid 40   and name HN  ))
  (( segid "BrD " and resid 42   and name HA  ))
   3 400     2 900     2 100 peak  4371 weight  0 10000E+01 volume  0.12104E+03 ppm1      8 662 ppm2      5 021
ASSI { 4671}
  (( segid "BrD " and resid 61   and name HN  ))
  (( segid "BrD " and resid 60   and name HB1 ))
   2 900     2 100     2 100 peak  4671 weight  0.10000E+01 volume  0 31176E+03 ppm1      8.746 ppm2      4 992
ASSI { 5081}
  (( segid "BrD " and resid 73   and name HN  ))
  (( segid "BrD " and resid 74   and name HB2 ))
   3 100     2 400     2 400 peak  5081 weight  0 10000E+01 volume  0 21337E+03 ppm1      8 007 ppm2      3 018
ASSI { 7641}
  (( segid "BrD " and resid 76   and name HN  ))
  (( segid "BrD " and resid 73   and name HA  ))
   3.500     3 100     2 000 peak  7641 weight  0 10000E+01 volume  0.97995E+02 ppm1      8 611 ppm2      4 812
ASSI { 7691}
  (( segid "BrD " and resid 83   and name HN  ))
  (( segid "BrD " and resid 80   and name HA  ))
   2 800     2 000     2 000 peak  7691 weight  0 10000E+01 volume  0.35765E+03 ppm1      9 660 ppm2      4.675
ASSI { 8061}
  (( segid "BrD " and resid 39   and name HN  ))
  (( segid "BrD " and resid 38   and name HN  ))
   4 300     4 300     1 200 peak  8061 weight  0 10000E+01 volume  0 29321E+02 ppm1      9 651 ppm2      8.726
ASSI { 8071}
  (( segid "BrD " and resid 39   and name HN  ))
  (( segid "BrD " and resid 42   and name HG1 ))
   4 100     4 100     1 400 peak  8071 weight  0 10000E+01 volume  0 37403E+02 ppm1      9 657 ppm2      2 891
ASSI { 8081}
  (( segid "BrD " and resid 39   and name HN  ))
  (( segid "BrD " and resid 42   and name HB1 ))
   3 900     3 800     1.600 peak  8081 weight  0 10000E+01 volume  0 55108E+02 ppm1      9.658 ppm2      2 784
ASSI { 8091}
  (( segid "BrD " and resid 39   and name HN  ))
  (( segid "BrD " and resid 42   and name HB2 ))
   4 200     4 200     1 300 peak  8091 weight  0 10000E+01 volume  0 33585E+02 ppm1      9 651 ppm2      2 607
ASSI { 8141}
  (( segid "BrD " and resid 57   and name HN  ))
  (( segid "BrD " and resid 36   and name HA  ))
   3 100     2 400     2 400 peak  8141 weight  0 10000E+01 volume  0 21622E+03 ppm1      9 359 ppm2      5 440
ASSI { 8151}
  (( segid "BrD " and resid 57   and name HN  ))
  (( segid "BrD " and resid 58   and name HA  ))
   4 100     4 100     1 400 peak  8151 weight  0 10000E+01 volume  0 38316E+02 ppm1      9 359 ppm2      4 453
ASSI { 8161}
  (( segid "BrD " and resid 57   and name HN  ))
  (( segid "BrD " and resid 37   and name HD1 ))
   3 700     3 400     1 800 peak  8161 weight  0 10000E+01 volume  0.78885E+02 ppm1      9 359 ppm2      4 288
ASSI { 8221}
  (( segid "BrD " and resid 114  and name HN  ))
  (( segid "BrD " and resid 115  and name HG  ))
   3 800     3 600     1 700 peak  8221 weight  0 10000E+01 volume  0 68239E+02 ppm1      8 377 ppm2      2 169
OR { 8221}
  (( segid "BrD " and resid 114  and name HN  ))
  (( segid "BrD " and resid 115  and name HB1 ))
ASSI { 8231}
  (( segid "BrD " and resid 114  and name HN  ))
  (  segid "BrD " and resid 115  and name HD1%)
   3 700     3 400     1.800 peak  8231 weight  0 10000E+01 volume  0 72638E+02 ppm1      8.375 ppm2      1 308
ASSI { 8271}
  (( segid "BrD " and resid 28   and name HN  ))
  (  segid "BrD " and resid 31   and name HB% )
   3 400     2.900     2 100 peak  8271 weight  0 10000E+01 volume  0 12341E+03 ppm1      8 166 ppm2      2 308
ASSI { 8281}
  (( segid "BrD " and resid 28   and name HN  ))
  (( segid "BrD " and resid 26   and name HB1 ))
   3 700     3 400     1 800 peak  8281 weight  0 10000E+01 volume  0 69844E+02 ppm1      8 166 ppm2      2 476
ASSI { 8301}
  (( segid "BrD " and resid 28   and name HN  ))
  (  segid "BrD " and resid 102  and name HD1%)
   3 400     2 900     2 100 peak  8301 weight  0 10000E+01 volume  0 11542E+03 ppm1      8.166 ppm2      1 318
ASSI { 8311}
  (( segid "BrD " and resid 118  and name HN  ))
  (( segid "BrD " and resid 116  and name HG12))
   3 200     2 600     2 300 peak  8311 weight  0 10000E+01 volume  0 19156E+03 ppm1      8.381 ppm2      1 558
ASSI { 8321}
  (( segid "BrD " and resid 118  and name HN  ))
  (  segid "BrD " and resid 116  and name HD1%)
   4 100     4 100     1.400 peak  8321 weight  0 10000E+01 volume  0.39844E+02 ppm1      8.380 ppm2      1 394
OR { 8321}
  (( segid "BrD " and resid 118  and name HN  ))
  (  segid "BrD " and resid 116  and name HG2%)
ASSI { 8331}
  (( segid "BrD " and resid 118  and name HN  ))
  (  segid "BrD " and resid 110  and name HG2%)
   3 400     2 900     2 100 peak  8331 weight  0.10000E+01 volume  0 11494E+03 ppm1      8 381 ppm2      1.296
ASSI { 8341}
  (( segid "BrD " and resid 51   and name HN  ))
  (  segid "BrD " and resid 50   and name HD1%)
   4 000     4 000     1 500 peak  8341 weight  0 10000E+01 volume  0 45762E+02 ppm1      8.381 ppm2      1 156
ASSI { 8401}
  (( segid "BrD " and resid 38   and name HN  ))
  (( segid "BrD " and resid 37   and name HB2 ))
   3 000     2 200     2 200 peak  8401 weight  0 10000E+01 volume  0.24692E+03 ppm1      8 733 ppm2      2 290
ASSI { 8411}
  (( segid "BrD " and resid 117  and name HN  ))
  (( segid "BrD " and resid 118  and name HN  ))
   3 900     3 800     1 600 peak  8411 weight  0 10000E+01 volume  0 55844E+02 ppm1      8 880 ppm2      8 368
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ASSI { 8421}
  (( segid "BrD " and resid 117  and name HN  ))
  (( segid "BrD " and resid 116  and name HG11))
     3 900     3 800     1 600 peak  8421 weight  0.10000E+01 volume  0.57435E+02 ppm1      8 876 ppm2      1 915
ASSI { 8441}
  (( segid "BrD " and resid 7    and name HN  ))
  (( segid "BrD " and resid 6    and name HD1 ))
     3 800     3 600     1 700 peak  8441 weight  0 10000E+01 volume  0 67409E+02 ppm1      8 923 ppm2      2 338
ASSI { 8451}
  (( segid "BrD " and resid 102  and name HN  ))
  (( segid "BrD " and resid 28   and name HE1 ))
     3 900     3 800     1 600 peak  8451 weight  0 10000E+01 volume  0 51665E+02 ppm1      9 156 ppm2      8 153
ASSI { 8461}
  (( segid "BrD " and resid 102  and name HN  ))
  (  segid "BrD " and resid 82   and name HE% )
     4 100     4 100     1 400 peak  8461 weight  0 10000E+01 volume  0 42485E+02 ppm1      9 156 ppm2      7 050
OR { 8461}
  (( segid "BrD " and resid 102  and name HN  ))
  (( segid "BrD " and resid 82   and name HZ  ))
ASSI { 8481}
  (( segid "BrD " and resid 102  and name HN  ))
  (( segid "BrD " and resid 103  and name HB1 ))
     3.600     3 200     1.900 peak  8481 weight  0 10000E+01 volume  0 86913E+02 ppm1      9 156 ppm2      2 348
ASSI { 8501}
  (( segid "BrD " and resid 50   and name HN  ))
  (( segid "BrD " and resid 48   and name HA  ))
     5 100     5 100     0 400 peak  8501 weight  0 10000E+01 volume  0 11267E+02 ppm1      8 564 ppm2      4 822
ASSI { 8551}
  (( segid "BrD " and resid 46   and name HN  ))
  (( segid "BrD " and resid 44   and name HA  ))
     4 000     4 000     1 500 peak  8551 weight  0 10000E+01 volume  0.43724E+02 ppm1      8 562 ppm2      5 119
ASSI { 8581}
  (( segid "BrD " and resid 46   and name HN  ))
  (  segid "BrD " and resid 43   and name HB% )
     2 800     2 000     2 000 peak  8581 weight  0 10000E+01 volume  0 40920E+03 ppm1      8.562 ppm2      1 692
ASSI { 8601}
  (( segid "BrD " and resid 43   and name HN  ))
  (( segid "BrD " and resid 39   and name HB1 ))
     4 100     4 100     1 400 peak  8601 weight  0 10000E+01 volume  0 39702E+02 ppm1      8 001 ppm2      2 497
ASSI { 8611}
  (( segid "BrD " and resid 43   and name HN  ))
  (( segid "BrD " and resid 39   and name HD1 ))
     3 500     3 100     2 000 peak  8611 weight  0 10000E+01 volume  0 96093E+02 ppm1      8 001 ppm2      2 292
ASSI { 8621}
  (( segid "BrD " and resid 43   and name HN  ))
  (  segid "BrD " and resid 41   and name HG2%)
     4 200     4 200     1 300 peak  8621 weight  0 10000E+01 volume  0.33897E+02 ppm1      8 001 ppm2      1 887
ASSI { 8631}
  (( segid "BrD " and resid 43   and name HN  ))
  (  segid "BrD " and resid 38   and name HG1%)
     4.300     4 300     1 200 peak  8631 weight  0 10000E+01 volume  0 32108E+02 ppm1      8 002 ppm2      1 058
ASSI { 8641}
  (( segid "BrD " and resid 43   and name HN  ))
  (  segid "BrD " and resid 38   and name HG2%)
     3 900     3 800     1 600 peak  8641 weight  0.10000E+01 volume  0 57231E+02 ppm1      8.001 ppm2      0 778
ASSI { 8661}
  (( segid "BrD " and resid 111  and name HN  ))
  (( segid "BrD " and resid 112  and name HB1 ))
     3 800     3 600     1 700 peak  8661 weight  0 10000E+01 volume  0 66898E+02 ppm1      8 167 ppm2      2 659
ASSI { 8681}
  (( segid "BrD " and resid 111  and name HN  ))
  (  segid "BrD " and resid 110  and name HG2%)
     3 000     2 200     2 200 peak  8681 weight  0 10000E+01 volume  0 28506E+03 ppm1      8 169 ppm2      1 250
ASSI { 8691}
  (( segid "BrD " and resid 111  and name HN  ))
  (  segid "BrD " and resid 116  and name HD1%)
     3 400     2 900     2 100 peak  8691 weight  0 10000E+01 volume  0 11425E+03 ppm1      8 168 ppm2      1 396
ASSI { 8711}
  (( segid "BrD " and resid 58   and name HN  ))
  (( segid "BrD " and resid 37   and name HD1 ))
     3 700     3 400     1 800 peak  8711 weight  0 10000E+01 volume  0 73156E+02 ppm1     10.051 ppm2      4 255
ASSI { 8721}
  (( segid "BrD " and resid 58   and name HN  ))
  (( segid "BrD " and resid 59   and name HG2 ))
     5 500     5 500     0 000 peak  8721 weight  0 10000E+01 volume  0 48442E+00 ppm1     10 051 ppm2      3 087
ASSI { 8801}
  (( segid "BrD " and resid 58   and name HN  ))
  (  segid "BrD " and resid 54   and name HE% )
     4 600     4 600     0 900 peak  8801 weight  0 10000E+01 volume  0 21191E+02 ppm1     10 050 ppm2      2.534
ASSI { 8971}
  (( segid "BrD " and resid 112  and name HN  ))
  (  segid "BrD " and resid 110  and name HG2%)
     3 800     3.600     1.700 peak  8971 weight  0 10000E+01 volume  0 60828E+02 ppm1      8 669 ppm2      1.263
ASSI { 8991}
  (( segid "BrD " and resid 105  and name HN  ))
  (( segid "BrD " and resid 106  and name HB1 ))
     3 500     3 100     2.000 peak  8991 weight  0 10000E+01 volume  0.10888E+03 ppm1      8 487 ppm2      3 870
ASSI { 9041}
  (( segid "BrD " and resid 105  and name HN  ))
  (  segid "BrD " and resid 102  and name HD2%)
     3 700     3 400     1.800 peak  9041 weight  0 10000E+01 volume  0 76403E+02 ppm1      8 486 ppm2      1 320
OR { 9041}
  (( segid "BrD " and resid 105  and name HN  ))
  (  segid "BrD " and resid 102  and name HD1%)
ASSI { 9051}
  (( segid "BrD " and resid 105  and name HN  ))
  (  segid "BrD " and resid 101  and name HG2%)
     3.900     3 800     1 600 peak  9051 weight  0 10000E+01 volume  0 50603E+02 ppm1      8.486 ppm2      1 602
ASSI { 9131}
  (( segid "BrD " and resid 21   and name HN  ))
  (( segid "BrD " and resid 21   and name HG12))
     3 200     2.600     2 300 peak  9131 weight  0.10000E+01 volume  0 17190E+03 ppm1      8 574 ppm2      1 620
OR { 9131}
  (( segid "BrD " and resid 21   and name HN  ))
  (  segid "BrD " and resid 21   and name HG2%)
ASSI { 9211}
  (( segid "BrD " and resid 106  and name HN  ))
  (  segid "BrD " and resid 102  and name HD2%)
     3 800     3 600     1 700 peak  9211 weight  0 10000E+01 volume  0 58744E+02 ppm1      9 740 ppm2      1 314
ASSI { 9221}
  (( segid "BrD " and resid 106  and name HN  ))
  (  segid "BrD " and resid 82   and name HE% )
     4 600     4 600     0 900 peak  9221 weight  0 10000E+01 volume  0 19539E+02 ppm1      9 740 ppm2      7 033
OR { 9221}
  (( segid "BrD " and resid 106  and name HN  ))
  (( segid "BrD " and resid 82   and name HZ  ))
ASSI { 9231}
  (( segid "BrD " and resid 84   and name HN  ))
  (( segid "BrD " and resid 80   and name HA  ))
     2 400     1.400     1 400 peak  9231 weight  0.10000E+01 volume  0 97923E+03 ppm1      9 464 ppm2      4 674
ASSI { 9261}
  (( segid "BrD " and resid 84   and name HN  ))
  (  segid "BrD " and resid 50   and name HD1%)
     4 700     4 700     0 800 peak  9261 weight  0.10000E+01 volume  0 17291E+02 ppm1      9 463 ppm2      1 136
ASSI { 9271}
  (( segid "BrD " and resid 84   and name HN  ))
  (  segid "BrD " and resid 50   and name HG2%)
     4.800     4 800     0.700 peak  9271 weight  0 10000E+01 volume  0 16063E+02 ppm1      9 464 ppm2      0 994
ASSI { 9381}
  (( segid "BrD " and resid 63   and name HN  ))
  (( segid "BrD " and resid 63   and name HB1 ))
     2.800     2 000     2 000 peak  9381 weight  0 10000E+01 volume  0 41354E+03 ppm1      9 456 ppm2      2 904
ASSI { 9411}
  (( segid "BrD " and resid 22   and name HN  ))
  (  segid "BrD " and resid 25   and name HG1%)
     3 600     3 200     1 900 peak  9411 weight  0 10000E+01 volume  0 92991E+02 ppm1      9 456 ppm2      1 797
ASSI { 9421}
  (( segid "BrD " and resid 22   and name HN  ))
  (  segid "BrD " and resid 21   and name HD1%)
     3 700     3 400     1 800 peak  9421 weight  0 10000E+01 volume  0 76602E+02 ppm1      9 456 ppm2      1.228
ASSI { 9431}
  (( segid "BrD " and resid 63   and name HN  ))
  (  segid "BrD " and resid 68   and name HD% )
     3.800     3 600     1 700 peak  9431 weight  0 10000E+01 volume  0 63643E+02 ppm1      9 456 ppm2      7.806
ASSI { 9481}
  (( segid "BrD " and resid 109  and name HN  ))
  (( segid "BrD " and resid 109  and name HD1 ))
     3 100     2 400     2 400 peak  9481 weight  0 10000E+01 volume  0 19915E+03 ppm1      8 556 ppm2      2 031
ASSI { 9521}
  (( segid "BrD " and resid 103  and name HN  ))
  (  segid "BrD " and resid 82   and name HE% )
     3 300     2 700     2 200 peak  9521 weight  0 10000E+01 volume  0 14888E+03 ppm1      8 695 ppm2      7 050
OR { 9521}
  (( segid "BrD " and resid 103  and name HN  ))
  (( segid "BrD " and resid 82   and name HZ  ))
ASSI { 9541}
  (( segid "BrD " and resid 112  and name HN  ))
  (( segid "BrD " and resid 111  and name HA  ))
     4 900     4 900     0 600 peak  9541 weight  0.10000E+01 volume  0 13131E+02 ppm1      8 696 ppm2      4 682
ASSI { 9611}
  (( segid "BrD " and resid 99   and name HN  ))
  (  segid "BrD " and resid 34   and name HE% )
     3 500     3 100     2 000 peak  9611 weight  0 10000E+01 volume  0 10701E+03 ppm1      8 936 ppm2      7 772
ASSI { 9671}
  (( segid "BrD " and resid 99   and name HN  ))
  (( segid "BrD " and resid 30   and name HB2 ))
     4 300     4 300     1 200 peak  9671 weight  0 10000E+01 volume  0 29603E+02 ppm1      8 936 ppm2      4.568
ASSI { 9681}
  (( segid "BrD " and resid 18   and name HN  ))
  (  segid "BrD " and resid 14   and name HD2%)
     3 600     3 200     1.900 peak  9681 weight  0 10000E+01 volume  0 80801E+02 ppm1      9 074 ppm2      1 390
OR { 9681}
  (( segid "BrD " and resid 18   and name HN  ))
  (  segid "BrD " and resid 14   and name HD1%)
ASSI { 9751}
  (( segid "BrD " and resid 64   and name HN  ))
  (( segid "BrD " and resid 63   and name HB2 ))
     2 400     1 400     1.400 peak  9751 weight  0.10000E+01 volume  0 10265E+04 ppm1      8 585 ppm2      2 532
ASSI { 9761}
  (( segid "BrD " and resid 64   and name HN  ))
  (  segid "BrD " and resid 63   and name HD2%)
     3 300     2 700     2 200 peak  9761 weight  0.10000E+01 volume  0 14024E+03 ppm1      8 585 ppm2      1 489
ASSI { 9811}
  (( segid "BrD " and resid 17   and name HN  ))
  (( segid "BrD " and resid 15   and name HB1 ))
     4 300     4 300     1.200 peak  9811 weight  0 10000E+01 volume  0 29691E+02 ppm1      8 669 ppm2      3 842
ASSI { 9851}
  (( segid "BrD " and resid 40   and name HN  ))
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   ( segid "BrD " and resid 41   and name HG2%)
     2.500     1.600    1.600 peak  9851 weight  0.10000E+01 volume  0.73405E+03 ppm1     8 669 ppm2     1 866
ASSI { 9871}
   (( segid "BrD " and resid 17   and name HN  ))
   (  segid "BrD " and resid 14   and name HD2%)
     4 000     4 000    1 500 peak  9871 weight  0 10000E+01 volume  0 46134E+02 ppm1     8.668 ppm2     1 379
OR { 9871}
   (( segid "BrD " and resid 17   and name HN  ))
   (  segid "BrD " and resid 14   and name HD1%)
ASSI { 9881}
   (( segid "BrD " and resid 17   and name HN  ))
   (  segid "BrD " and resid 18   and name HD2%)
     4 600     4 600    0 900 peak  9881 weight  0 10000E+01 volume  0 20602E+02 ppm1     8.669 ppm2     0 394
ASSI { 9911}
   (( segid "BrD " and resid 72   and name HN  ))
   (( segid "BrD " and resid 73   and name HB2 ))
     3 000     2 200    2 200 peak  9911 weight  0 10000E+01 volume  0 24469E+03 ppm1     8 858 ppm2     2 503
ASSI { 9951}
   (( segid "BrD " and resid 12   and name HN  ))
   (( segid "BrD " and resid 13   and name HA  ))
     3 800     3 600    1 700 peak  9951 weight  0 10000E+01 volume  0 59337E+02 ppm1     9 021 ppm2     4 770
ASSI { 9971}
   (( segid "BrD " and resid 12   and name HN  ))
   (( segid "BrD " and resid 15   and name HB2 ))
     4 100     4.100    1 400 peak  9971 weight  0 10000E+01 volume  0 38398E+02 ppm1     9.021 ppm2     3 618
ASSI { 9981}
   (( segid "BrD " and resid 12   and name HN  ))
   (( segid "BrD " and resid 11   and name HB1 ))
     3 200     2 600    2 300 peak  9981 weight  0 10000E+01 volume  0 16530E+03 ppm1     9 021 ppm2     2 971
ASSI { 9991}
   (( segid "BrD " and resid 12   and name HN  ))
   (( segid "BrD " and resid 11   and name HB2 ))
     3.300     2 700    2 200 peak  9991 weight  0 10000E+01 volume  0 13633E+03 ppm1     9 022 ppm2     2 611
OR { 9991}
   (( segid "BrD " and resid 12   and name HN  ))
   (( segid "BrD " and resid 11   and name HG1 ))
ASSI {10021}
   (( segid "BrD " and resid 25   and name HN  ))
   (( segid "BrD " and resid 26   and name HD1 ))
     3 700     3 400    1 800 peak 10021 weight  0 10000E+01 volume  0 71669E+02 ppm1     9 134 ppm2     2 092
ASSI {10031}
   (( segid "BrD " and resid 25   and name HN  ))
   (  segid "BrD " and resid 102  and name HD1%)
     3 800     3 600    1 700 peak 10031 weight  0 10000E+01 volume  0 60868E+02 ppm1     9 133 ppm2     1 295
OR {10031}
   (( segid "BrD " and resid 25   and name HN  ))
   (  segid "BrD " and resid 102  and name HD2%)
ASSI {10061}
   (( segid "BrD " and resid 24   and name HN  ))
   (  segid "BrD " and resid 25   and name HG1%)
     3 600     3 200    1 900 peak 10061 weight  0 10000E+01 volume  0 91063E+02 ppm1     8 657 ppm2     1 798
ASSI {10191}
   (( segid "BrD " and resid 16   and name HN  ))
   (( segid "BrD " and resid 18   and name HG  ))
     3 700     3 400    1.800 peak 10191 weight  0 10000E+01 volume  0 73953E+02 ppm1     8 792 ppm2     2 295
ASSI {10221}
   (( segid "BrD " and resid 76   and name HN  ))
   (( segid "BrD " and resid 74   and name HN  ))
     3 300     2.700    2 200 peak 10221 weight  0 10000E+01 volume  0 15827E+03 ppm1     8 611 ppm2     7 532
ASSI {10251}
   (( segid "BrD " and resid 75   and name HN  ))
   (  segid "BrD " and resid 18   and name HD1%)
     4.200     4 200    1 300 peak 10251 weight  0 10000E+01 volume  0 32785E+02 ppm1     9.105 ppm2     1 056
ASSI {10261}
   (( segid "BrD " and resid 75   and name HN  ))
   (  segid "BrD " and resid 76   and name HB% )
     3 400     2 900    2 100 peak 10261 weight  0.10000E+01 volume  0 13102E+03 ppm1     9 106 ppm2     2 099
ASSI {10291}
   (( segid "BrD " and resid 75   and name HN  ))
   (  segid "BrD " and resid 75   and name HE% )
     3 800     3 600    1 700 peak 10291 weight  0 10000E+01 volume  0 67546E+02 ppm1     9 108 ppm2     2 654
ASSI {10301}
   (( segid "BrD " and resid 75   and name HN  ))
   (  segid "BrD " and resid 18   and name HD2%)
     3 900     3.800    1 600 peak 10301 weight  0 10000E+01 volume  0.57563E+02 ppm1     9 106 ppm2     0 429
ASSI {10351}
   (( segid "BrD " and resid 95   and name HN  ))
   (( segid "BrD " and resid 93   and name HB1 ))
     2.900     2 100    2.100 peak 10351 weight  0 10000E+01 volume  0 35043E+03 ppm1     8 669 ppm2     5 018
ASSI {10401}
   (( segid "BrD " and resid 55   and name HN  ))
   (( segid "BrD " and resid 37   and name HB2 ))
     3 600     3 200    1 900 peak 10401 weight  0 10000E+01 volume  0 94850E+02 ppm1     7 996 ppm2     2 295
ASSI {10421}
   (( segid "BrD " and resid 55   and name HN  ))
   (( segid "BrD " and resid 37   and name HG2 ))
     2 700     1 800    1.800 peak 10421 weight  0 10000E+01 volume  0 46013E+03 ppm1     7 996 ppm2     2 578
ASSI {10441}
   (( segid "BrD " and resid 96   and name HN  ))
   (( segid "BrD " and resid 95   and name HB1 ))
     3 300     2 700    2 200 peak 10441 weight  0.10000E+01 volume  0 14200E+03 ppm1     7 988 ppm2     3 587
ASSI {10571}
   (( segid "BrD " and resid 80   and name HN  ))
   (( segid "BrD " and resid 79   and name HG1 ))
     2.400     1.400    1.400 peak 10571 weight  0.10000E+01 volume  0.10119E+04 ppm1     7 975 ppm2     3 105
ASSI {10581}
   (( segid "BrD " and resid 78   and name HN  ))
   (( segid "BrD " and resid 77   and name HB1 ))
     3 000     2 200    2 200 peak 10581 weight  0 10000E+01 volume  0 26376E+03 ppm1     7 974 ppm2     3.301
ASSI {10591}
   (( segid "BrD " and resid 55   and name HN  ))
   (( segid "BrD " and resid 58   and name HN  ))
     4 100     4 100    1 400 peak 10591 weight  0 10000E+01 volume  0 42990E+02 ppm1     7 972 ppm2     10 062
ASSI {10621}
   (( segid "BrD " and resid 56   and name HN  ))
   (( segid "BrD " and resid 34   and name HB1 ))
     3 700     3 400    1 800 peak 10621 weight  0.10000E+01 volume  0 69879E+02 ppm1     9 674 ppm2     4 100
ASSI {10641}
   (( segid "BrD " and resid 82   and name HN  ))
   (( segid "BrD " and resid 80   and name HB1 ))
     4 200     4 200    1 300 peak 10641 weight  0 10000E+01 volume  0 33240E+02 ppm1     6 981 ppm2     2 603
ASSI {10651}
   (( segid "BrD " and resid 82   and name HN  ))
   (( segid "BrD " and resid 84   and name HB2 ))
     4 300     4 300    1 200 peak 10651 weight  0 10000E+01 volume  0 31962E+02 ppm1     6 981 ppm2     3 230
ASSI {10661}
   (( segid "BrD " and resid 82   and name HN  ))
   (  segid "BrD " and resid 99   and name HB% )
     4 100     4 100    1 400 peak 10661 weight  0.10000E+01 volume  0 41756E+02 ppm1     6 981 ppm2     2 202
ASSI {10721}
   (( segid "BrD " and resid 81   and name HN  ))
   (( segid "BrD " and resid 77   and name HB1 ))
     3 900     3 800    1 600 peak 10721 weight  0 10000E+01 volume  0 54085E+02 ppm1     7 641 ppm2     3 310
ASSI {10751}
   (( segid "BrD " and resid 80   and name HN  ))
   (( segid "BrD " and resid 77   and name HB1 ))
     4 400     4 400    1 100 peak 10751 weight  0 10000E+01 volume  0 26321E+02 ppm1     8 005 ppm2     3 322
ASSI {10771}
   (( segid "BrD " and resid 80   and name HN  ))
   (( segid "BrD " and resid 81   and name HB  ))
     3 700     3 400    1 800 peak 10771 weight  0.10000E+01 volume  0 71103E+02 ppm1     8 006 ppm2     2 049
ASSI {10841}
   (( segid "BrD " and resid 79   and name HN  ))
   (  segid "BrD " and resid 76   and name HB% )
     3 500     3 100    2 000 peak 10841 weight  0 10000E+01 volume  0 10580E+03 ppm1     8 681 ppm2     2 096
ASSI {10881}
   (( segid "BrD " and resid 85   and name HN  ))
   (  segid "BrD " and resid 99   and name HB% )
     3 900     3 800    1 600 peak 10881 weight  0.10000E+01 volume  0 56660E+02 ppm1     7 515 ppm2     2 208
ASSI {10891}
   (( segid "BrD " and resid 85   and name HN  ))
   (  segid "BrD " and resid 81   and name HG2%)
     4 100     4 100    1 400 peak 10891 weight  0 10000E+01 volume  0 42261E+02 ppm1     7 522 ppm2     0 765
ASSI {10921}
   (( segid "BrD " and resid 86   and name HN  ))
   (( segid "BrD " and resid 87   and name HB1 ))
     3 800     3 600    1 700 peak 10921 weight  0 10000E+01 volume  0 59880E+02 ppm1     8 423 ppm2     2 779
OR {10921}
   (( segid "BrD " and resid 86   and name HN  ))
   (( segid "BrD " and resid 87   and name HG2 ))
ASSI {10931}
   (( segid "BrD " and resid 86   and name HN  ))
   (( segid "BrD " and resid 87   and name HB2 ))
     3 800     3 600    1 700 peak 10931 weight  0 10000E+01 volume  0 59561E+02 ppm1     8.423 ppm2     2.577
ASSI {10941}
   (( segid "BrD " and resid 86   and name HN  ))
   (  segid "BrD " and resid 99   and name HB% )
     3 600     3 200    1 900 peak 10941 weight  0 10000E+01 volume  0 93545E+02 ppm1     8.423 ppm2     2 210
ASSI {11001}
   (( segid "BrD " and resid 87   and name HN  ))
   (  segid "BrD " and resid 50   and name HD1%)
     3 800     3 600    1 700 peak 11001 weight  0 10000E+01 volume  0 61476E+02 ppm1     8 570 ppm2     1 148
ASSI {11021}
   (( segid "BrD " and resid 87   and name HN  ))
   (( segid "BrD " and resid 86   and name HG2 ))
     4 500     4 500    1 000 peak 11021 weight  0 10000E+01 volume  0 22088E+02 ppm1     8 571 ppm2     0 780
ASSI {11031}
   (( segid "BrD " and resid 88   and name HN  ))
   (  segid "BrD " and resid 50   and name HD1%)
     3.600     3 200    1 900 peak 11031 weight  0 10000E+01 volume  0.90228E+02 ppm1     8 354 ppm2     1 146
ASSI {11041}
   (( segid "BrD " and resid 88   and name HN  ))
   (( segid "BrD " and resid 84   and name HB2 ))
     4 000     4 000    1 500 peak 11041 weight  0 10000E+01 volume  0 46286E+02 ppm1     8.354 ppm2     3 299
ASSI {11051}
   (( segid "BrD " and resid 88   and name HN  ))
   (( segid "BrD " and resid 87   and name HG1 ))
     4 600     4 600    0.900 peak 11051 weight  0 10000E+01 volume  0 19886E+02 ppm1     8 354 ppm2     3 018
ASSI {11161}
   (( segid "BrD " and resid 93   and name HN  ))
   (( segid "BrD " and resid 91   and name HD2 ))
     3 700     3 400    1 800 peak 11161 weight  0.10000E+01 volume  0 78354E+02 ppm1     8 714 ppm2     4 410
ASSI {11171}
   (( segid "BrD " and resid 93   and name HN  ))
   (( segid "BrD " and resid 96   and name HB1 ))
     3 300     2 700    2 200 peak 11171 weight  0 10000E+01 volume  0 14983E+03 ppm1     8 714 ppm2     4 004
ASSI {11191}
   (( segid "BrD " and resid 30   and name HN  ))
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  (( segid "BrD " and resid 28   and name HB2 ))
     4.400     4.400      1.100 peak 11191 weight  0.10000E+01 volume  0.26154E+02 ppm1     12.276 ppm2     3.392
ASSI {11201}
  (( segid "BrD " and resid 30   and name HN  ))
  (( segid "BrD " and resid 28   and name HB1 ))
     3 300     2 700      2 200 peak 11201 weight  0 10000E+01 volume  0.15024E+03 ppm1     12 275 ppm2     3 594
ASSI {11211}
  (( segid "BrD " and resid 30   and name HN  ))
  (( segid "BrD " and resid 32   and name HN  ))
     3 600     3 200      1 900 peak 11211 weight  0 10000E+01 volume  0 82022E+02 ppm1     12 276 ppm2     7 741
ASSI {11241}
  (( segid "BrD " and resid 31   and name HN  ))
  (( segid "BrD " and resid 28   and name HB1 ))
     3 600     3 200      1 900 peak 11241 weight  0 10000E+01 volume  0 94685E+02 ppm1     8 480 ppm2      3 594
ASSI {11251}
  (( segid "BrD " and resid 31   and name HN  ))
  (( segid "BrD " and resid 28   and name HB2 ))
     3 800     3 600      1 700 peak 11251 weight  0 10000E+01 volume  0 64760E+02 ppm1     8 481 ppm2      3 389
ASSI {11361}
  (( segid "BrD " and resid 32   and name HN  ))
  (  segid "BrD " and resid 102  and name HD1%)
     4 500     4 500      1 000 peak 11361 weight  0 10000E+01 volume  0 23592E+02 ppm1     7 738 ppm2      1 310
ASSI {11391}
  (( segid "BrD " and resid 34   and name HN  ))
  (( segid "BrD " and resid 35   and name HG1 ))
     3 200     2 600      2 300 peak 11391 weight  0 10000E+01 volume  0 18521E+03 ppm1     8 182 ppm2      3 447
ASSI {11431}
  (( segid "BrD " and resid 34   and name HN  ))
  (  segid "BrD " and resid 31   and name HB% )
     2 900     2 100      2 100 peak 11431 weight  0 10000E+01 volume  0 29794E+03 ppm1     8 179 ppm2      2 301
ASSI {11441}
  (( segid "BrD " and resid 34   and name HN  ))
  (  segid "BrD " and resid 56   and name HD1%)
     3 400     2 900      2 100 peak 11441 weight  0 10000E+01 volume  0 12961E+03 ppm1     8 184 ppm2      1 527
ASSI {11451}
  (( segid "BrD " and resid 34   and name HN  ))
  (  segid "BrD " and resid 102  and name HD1%)
     3 600     3 200      1 900 peak 11451 weight  0 10000E+01 volume  0 84106E+02 ppm1     8 185 ppm2      1 305
ASSI {11521}
  (( segid "BrD " and resid 35   and name HN  ))
  (  segid "BrD " and resid 56   and name HD1%)
     4 500     4.500      1 000 peak 11521 weight  0.10000E+01 volume  0.22012E+02 ppm1     7 734 ppm2      1 553
ASSI {11561}
  (( segid "BrD " and resid 36   and name HN  ))
  (( segid "BrD " and resid 57   and name HB1 ))
     3 400     2 900      2 100 peak 11561 weight  0 10000E+01 volume  0 11642E+03 ppm1     8 308 ppm2      2 953
ASSI {11571}
  (( segid "BrD " and resid 66   and name HN  ))
  (  segid "BrD " and resid 63   and name HD1%)
     4 200     4 200      1 300 peak 11571 weight  0 10000E+01 volume  0 34773E+02 ppm1     8 763 ppm2      1 640
ASSI {11601}
  (( segid "BrD " and resid 67   and name HN  ))
  (  segid "BrD " and resid 68   and name HD% )
     4 400     4 400      1 100 peak 11601 weight  0 10000E+01 volume  0 26280E+02 ppm1     8 832 ppm2      7 780
ASSI {11651}
  (( segid "BrD " and resid 68   and name HN  ))
  (( segid "BrD " and resid 69   and name HB  ))
     3 700     3 400      1 800 peak 11651 weight  0.10000E+01 volume  0.74566E+02 ppm1     8 626 ppm2      2 947
ASSI {11661}
  (( segid "BrD " and resid 68   and name HN  ))
  (  segid "BrD " and resid 18   and name HD1%)
     5 500     5 500      0 000 peak 11661 weight  0 10000E+01 volume  0 40212E+01 ppm1     8 626 ppm2      1 090
ASSI {11731}
  (( segid "BrD " and resid 70   and name HN  ))
  (( segid "BrD " and resid 68   and name HB1 ))
     3 600     3 200      1 900 peak 11731 weight  0 10000E+01 volume  0 91804E+02 ppm1     8 040 ppm2      3 689
ASSI {11741}
  (( segid "BrD " and resid 70   and name HN  ))
  (( segid "BrD " and resid 74   and name HB1 ))
     3 400     2 900      2 100 peak 11741 weight  0 10000E+01 volume  0 13333E+03 ppm1     8 039 ppm2      3 544
ASSI {11771}
  (( segid "BrD " and resid 70   and name HN  ))
  (( segid "BrD " and resid 73   and name HB2 ))
     3 700     3 400      1 800 peak 11771 weight  0 10000E+01 volume  0 79558E+02 ppm1     8 040 ppm2      2 491
ASSI {11841}
  (( segid "BrD " and resid 73   and name HN  ))
  (( segid "BrD " and resid 70   and name HB2 ))
     3 200     2 600      2 300 peak 11841 weight  0.10000E+01 volume  0 16883E+03 ppm1     8 047 ppm2      4 361
ASSI {11891}
  (( segid "BrD " and resid 74   and name HN  ))
  (( segid "BrD " and resid 75   and name HB2 ))
     4 700     4 700      0.800 peak 11891 weight  0.10000E+01 volume  0 18157E+02 ppm1     7 536 ppm2      2 851
ASSI {11911}
  (( segid "BrD " and resid 74   and name HN  ))
  (  segid "BrD " and resid 76   and name HB% )
     4 400     4 400      1.100 peak 11911 weight  0.10000E+01 volume  0 27875E+02 ppm1     7.536 ppm2      2.088
ASSI {12031}
  (( segid "BrD " and resid 99   and name HN  ))
  (( segid "BrD " and resid 100  and name HB2 ))
     3 800     3 600      1.700 peak 12031 weight  0 10000E+01 volume  0.61845E+02 ppm1     8.936 ppm2      3 439
ASSI {12041}
  (( segid "BrD " and resid 99   and name HN  ))
  (( segid "BrD " and resid 97   and name HB1 ))
     3 400     2 900      2 100 peak 12041 weight  0 10000E+01 volume  0 12562E+03 ppm1     8 936 ppm2      2 721
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ASSI {12061}
  (( segid "BrD " and resid 100  and name HN  ))
  (( segid "BrD " and resid 101  and name HA  ))
     4 000     4.000      1 500 peak 12061 weight  0 10000E+01 volume  0.47923E+02 ppm1     8 669 ppm2      4 255
ASSI {12091}
  (( segid "BrD " and resid 100  and name HN  ))
  (( segid "BrD " and resid 101  and name HG11))
     4 100     4 100      1 400 peak 12091 weight  0 10000E+01 volume  0 39843E+02 ppm1     8 669 ppm2      2 519
OR {12091}
  (( segid "BrD " and resid 100  and name HN  ))
  (( segid "BrD " and resid 101  and name HB  ))
ASSI {12151}
  (( segid "BrD " and resid 101  and name HN  ))
  (( segid "BrD " and resid 104  and name HD1 ))
     3.500     3 100      2 000 peak 12151 weight  0 10000E+01 volume  0 11138E+03 ppm1     8 513 ppm2      2 282
ASSI {12221}
  (( segid "BrD " and resid 107  and name HN  ))
  (  segid "BrD " and resid 106  and name HD% )
     3.300     2 700      2 200 peak 12221 weight  0 10000E+01 volume  0 14273E+03 ppm1     8 981 ppm2      7 515
ASSI {12241}
  (( segid "BrD " and resid 107  and name HN  ))
  (( segid "BrD " and resid 103  and name HG2 ))
     3.400     2 900      2 100 peak 12241 weight  0 10000E+01 volume  0 11969E+03 ppm1     8 980 ppm2      2 547
ASSI {12271}
  (( segid "BrD " and resid 107  and name HN  ))
  (( segid "BrD " and resid 110  and name HG12))
     4 000     4 000      1 500 peak 12271 weight  0 10000E+01 volume  0 48486E+02 ppm1     8 980 ppm2      1 678
ASSI {12291}
  (( segid "BrD " and resid 108  and name HN  ))
  (( segid "BrD " and resid 109  and name HB2 ))
     5.500     5 500      0 000 peak 12291 weight  0 10000E+01 volume  0 20202E+00 ppm1     8 522 ppm2      2 195
ASSI {12411}
  (( segid "BrD " and resid 113  and name HN  ))
  (  segid "BrD " and resid 17   and name HG2%)
     4 300     4 300      1 200 peak 12411 weight  0 10000E+01 volume  0 28750E+02 ppm1     8 218 ppm2      1 728
ASSI {12431}
  (( segid "BrD " and resid 113  and name HN  ))
  (  segid "BrD " and resid 110  and name HG2%)
     3 400     2 900      2 100 peak 12431 weight  0 10000E+01 volume  0 12771E+03 ppm1     8 218 ppm2      1 275
ASSI {12441}
  (( segid "BrD " and resid 115  and name HN  ))
  (  segid "BrD " and resid 113  and name HB% )
     3 400     2 900      2 100 peak 12441 weight  0 10000E+01 volume  0.11633E+03 ppm1     8 355 ppm2      1 969
ASSI {12451}
  (( segid "BrD " and resid 115  and name HN  ))
  (( segid "BrD " and resid 116  and name HG12))
     5 500     5 500      0.000 peak 12451 weight  0 10000E+01 volume  0 47664E+01 ppm1     8 355 ppm2      1 558
ASSI {12461}
  (( segid "BrD " and resid 115  and name HN  ))
  (  segid "BrD " and resid 110  and name HD1%)
     4 400     4 400      1.100 peak 12461 weight  0 10000E+01 volume  0 26420E+02 ppm1     8 356 ppm2      1 163
ASSI {12471}
  (( segid "BrD " and resid 115  and name HN  ))
  (( segid "BrD " and resid 110  and name HB  ))
     3.700     3.400      1 800 peak 12471 weight  0 10000E+01 volume  0 76081E+02 ppm1     8 355 ppm2      2 346
ASSI {12481}
  (( segid "BrD " and resid 117  and name HN  ))
  (( segid "BrD " and resid 116  and name HG12))
     4 700     4.700      0 800 peak 12481 weight  0 10000E+01 volume  0 17262E+02 ppm1     8 883 ppm2      1 544
ASSI {12491}
  (( segid "BrD " and resid 116  and name HN  ))
  (  segid "BrD " and resid 110  and name HG2%)
     3.200     2 600      2 300 peak 12491 weight  0.10000E+01 volume  0 16590E+03 ppm1     8 083 ppm2      1 277
ASSI {12521}
  (( segid "BrD " and resid 116  and name HN  ))
  (  segid "BrD " and resid 110  and name HD1%)
     3.200     2 600      2 300 peak 12521 weight  0 10000E+01 volume  0.17496E+03 ppm1     8 086 ppm2      1 156
ASSI {12591}
  (( segid "BrD " and resid 47   and name HN  ))
  (( segid "BrD " and resid 48   and name HG2 ))
     4 200     4 200      1 300 peak 12591 weight  0 10000E+01 volume  0 33544E+02 ppm1     8 832 ppm2      2.861
ASSI {12611}
  (( segid "BrD " and resid 47   and name HN  ))
  (  segid "BrD " and resid 43   and name HB% )
     3 800     3.600      1 700 peak 12611 weight  0 10000E+01 volume  0 60519E+02 ppm1     8 832 ppm2      1 700
ASSI {12621}
  (( segid "BrD " and resid 49   and name HN  ))
  (( segid "BrD " and resid 50   and name HB  ))
     3 600     3.200      1 900 peak 12621 weight  0 10000E+01 volume  0 90984E+02 ppm1     7 762 ppm2      1 797
ASSI {12701}
  (( segid "BrD " and resid 52   and name HN  ))
  (( segid "BrD " and resid 53   and name HG1 ))
     3 900     3 800      1 600 peak 12701 weight  0 10000E+01 volume  0.53690E+02 ppm1     9 004 ppm2      2 820
OR {12701}
  (( segid "BrD " and resid 52   and name HN  ))
  (( segid "BrD " and resid 53   and name HB1 ))
ASSI {12741}
  (( segid "BrD " and resid 42   and name HN  ))
  (( segid "BrD " and resid 39   and name HB1 ))
     3 100     2.400      2 400 peak 12741 weight  0.10000E+01 volume  0.21408E+03 ppm1     7 820 ppm2      2 491
ASSI {12751}
  (( segid "BrD " and resid 42   and name HN  ))
  (( segid "BrD " and resid 39   and name HD1 ))
     3 000     2 200      2 200 peak 12751 weight  0 10000E+01 volume  0 25898E+03 ppm1     7 821 ppm2      2.286
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ASSI {12761}
  (( segid "BrD " and resid 42   and name HN  ))
  (  segid "BrD " and resid 43   and name HB% )
    3 500     3 100     2 000 peak 12761 weight  0 10000E+01 volume  0 10310E+03 ppm1      7 820 ppm2      1 706
ASSI {12851}
  (( segid "BrD " and resid 20   and name HN  ))
  (( segid "BrD " and resid 19   and name HD1 ))
    3 600     3 200     1 900 peak 12851 weight  0 10000E+01 volume  0 82185E+02 ppm1      8 145 ppm2      2 189
ASSI {12881}
  (( segid "BrD " and resid 20   and name HN  ))
  (( segid "BrD " and resid 21   and name HG12))
    3 900     3.800     1.600 peak 12881 weight  0 10000E+01 volume  0 55288E+02 ppm1      8 147 ppm2      1 639
OR {12881}
  (( segid "BrD " and resid 20   and name HN  ))
  (  segid "BrD " and resid 21   and name HG2%)
ASSI {12891}
  (( segid "BrD " and resid 20   and name HN  ))
  (  segid "BrD " and resid 63   and name HD2%)
    3 500     3 100     2 000 peak 12891 weight  0 10000E+01 volume  0 11141E+03 ppm1      8 146 ppm2      1.480
ASSI {12901}
  (( segid "BrD " and resid 20   and name HN  ))
  (  segid "BrD " and resid 17   and name HG2%)
    3 900     3.800     1 600 peak 12901 weight  0 10000E+01 volume  0 53573E+02 ppm1      8 146 ppm2      1 762
ASSI {12991}
  (( segid "BrD " and resid 23   and name HN  ))
  (( segid "BrD " and resid 20   and name HN  ))
    3 800     3 600     1 700 peak 12991 weight  0 10000E+01 volume  0 61946E+02 ppm1      9 119 ppm2      8 121
ASSI {13021}
  (( segid "BrD " and resid 26   and name HN  ))
  (( segid "BrD " and resid 28   and name HB2 ))
    4 200     4 200     1 300 peak 13021 weight  0 10000E+01 volume  0 33211E+02 ppm1      9 196 ppm2      3.393
ASSI {13031}
  (( segid "BrD " and resid 26   and name HN  ))
  (( segid "BrD " and resid 35   and name HG1 ))
    4 500     4 500     1 000 peak 13031 weight  0 10000E+01 volume  0 21672E+02 ppm1      9 195 ppm2      3 493
ASSI {13041}
  (( segid "BrD " and resid 26   and name HN  ))
  (  segid "BrD " and resid 56   and name HD2%)
    4.100     4 100     1 400 peak 13041 weight  0 10000E+01 volume  0 41596E+02 ppm1      9.196 ppm2      1 250
ASSI {13061}
  (( segid "BrD " and resid 27   and name HN  ))
  (( segid "BrD " and resid 26   and name HG1 ))
    3 800     3 600     1 700 peak 13061 weight  0 10000E+01 volume  0 66585E+02 ppm1      8 169 ppm2      1 596
ASSI {13091}
  (( segid "BrD " and resid 27   and name HN  ))
  (  segid "BrD " and resid 35   and name HE% )
    3 600     3 200     1 900 peak 13091 weight  0 10000E+01 volume  0 88198E+02 ppm1      8 169 ppm2      2 809
ASSI {13111}
  (( segid "BrD " and resid 59   and name HN  ))
  (  segid "BrD " and resid 59   and name HE% )
    3 300     2.700     2 200 peak 13111 weight  0 10000E+01 volume  0 15860E+03 ppm1      8 498 ppm2      1 864
ASSI {13131}
  (( segid "BrD " and resid 59   and name HN  ))
  (  segid "BrD " and resid 56   and name HD2%)
    4 300     4 300     1 200 peak 13131 weight  0 10000E+01 volume  0 28520E+02 ppm1      8 499 ppm2      1 239
ASSI {13161}
  (( segid "BrD " and resid 60   and name HN  ))
  (( segid "BrD " and resid 59   and name HG1 ))
    3 600     3 200     1 900 peak 13161 weight  0 10000E+01 volume  0.93397E+02 ppm1      8 565 ppm2      3 213
ASSI {13221}
  (( segid "BrD " and resid 32   and name HE1 ))
  (( segid "BrD " and resid 32   and name HD1 ))
    2 300     1 300     1 300 peak 13221 weight  0 10000E+01 volume  0.12506E+04 ppm1     11 082 ppm2      8 475
ASSI {13231}
  (( segid "BrD " and resid 32   and name HE1 ))
  (( segid "BrD " and resid 32   and name HN  ))
    3 200     2.600     2 300 peak 13231 weight  0 10000E+01 volume  0 18835E+03 ppm1     11.082 ppm2      7 742
OR {13231}
  (( segid "BrD " and resid 32   and name HE1 ))
  (( segid "BrD " and resid 32   and name HH2 ))
ASSI {13241}
  (( segid "BrD " and resid 32   and name HE1 ))
  (( segid "BrD " and resid 32   and name HZ2 ))
    2 500     1 600     1 600 peak 13241 weight  0 10000E+01 volume  0.70734E+03 ppm1     11 082 ppm2      7.984
ASSI {13251}
  (( segid "BrD " and resid 32   and name HE1 ))
  (( segid "BrD " and resid 30   and name HA  ))
    3 100     2 400     2.400 peak 13251 weight  0 10000E+01 volume  0 22949E+03 ppm1     11.082 ppm2      5 450
ASSI {13301}
  (( segid "BrD " and resid 76   and name HN  ))
  (( segid "BrD " and resid 77   and name HA  ))
    4 200     4 200     1 300 peak 13301 weight  0 10000E+01 volume  0 33586E+02 ppm1      8.610 ppm2      4 967
ASSI {13311}
  (( segid "BrD " and resid 76   and name HN  ))
  (( segid "BrD " and resid 77   and name HB1 ))
    4 100     4 100     1 400 peak 13311 weight  0 10000E+01 volume  0.37785E+02 ppm1      8.613 ppm2      3 344
ASSI {13651}
  (( segid "BrD " and resid 56   and name HN  ))
  (  segid "BrD " and resid 81   and name HG1%)
    4 100     4 100     1.400 peak 13651 weight  0 10000E+01 volume  0 38100E+02 ppm1      9 680 ppm2      1 077
ASSI {13661}
  (( segid "BrD " and resid 56   and name HN  ))
  (  segid "BrD " and resid 81   and name HG2%)
    4 200     4 200     1 300 peak 13661 weight  0.10000E+01 volume  0 33875E+02 ppm1      9 681 ppm2      0 743
ASSI {13681}
  (( segid "BrD " and resid 74   and name HN  ))
  (  segid "BrD " and resid 14   and name HD1%)
    4 700     4 700     0 800 peak 13681 weight  0 10000E+01 volume  0 17399E+02 ppm1      7 536 ppm2      1 405
OR {13681}
  (( segid "BrD " and resid 74   and name HN  ))
  (  segid "BrD " and resid 14   and name HD2%)
ASSI {13721}
  (( segid "BrD " and resid 16   and name HN  ))
  (( segid "BrD " and resid 17   and name HB  ))
    4.400     4 400     1 100 peak 13721 weight  0 10000E+01 volume  0 26713E+02 ppm1      8 794 ppm2      4 874
ASSI {13751}
  (( segid "BrD " and resid 74   and name HN  ))
  (( segid "BrD " and resid 68   and name HA  ))
    5.300     5 300     0 200 peak 13751 weight  0 10000E+01 volume  0.81254E+01 ppm1      7 537 ppm2      5 140
ASSI {13881}
  (( segid "BrD " and resid 46   and name HN  ))
  (  segid "BrD " and resid 38   and name HG1%)
    4 600     4 600     0 900 peak 13881 weight  0 10000E+01 volume  0 18836E+02 ppm1      8 562 ppm2      1 082
ASSI {13891}
  (( segid "BrD " and resid 62   and name HN  ))
  (( segid "BrD " and resid 67   and name HB1 ))
    4.100     4 100     1 400 peak 13891 weight  0 10000E+01 volume  0 40043E+02 ppm1      8 998 ppm2      3 557
ASSI {13931}
  (( segid "BrD " and resid 116  and name HN  ))
  (  segid "BrD " and resid 75   and name HE% )
    5 000     5 000     0 500 peak 13931 weight  0.10000E+01 volume  0 12168E+02 ppm1      8.086 ppm2      2 648
ASSI {13941}
  (( segid "BrD " and resid 115  and name HN  ))
  (( segid "BrD " and resid 110  and name HA  ))
    4 100     4 100     1 400 peak 13941 weight  0 10000E+01 volume  0.38338E+02 ppm1      8 355 ppm2      4 419
ASSI {13951}
  (( segid "BrD " and resid 114  and name HN  ))
  (( segid "BrD " and resid 112  and name HN  ))
    4 000     4 000     1 500 peak 13951 weight  0 10000E+01 volume  0 49230E+02 ppm1      8 375 ppm2      8.642
ASSI {13961}
  (( segid "BrD " and resid 114  and name HN  ))
  (( segid "BrD " and resid 112  and name HB1 ))
    5.200     5 200     0.300 peak 13961 weight  0 10000E+01 volume  0 99997E+01 ppm1      8 377 ppm2      2 665
ASSI {14001}
  (( segid "BrD " and resid 108  and name HN  ))
  (( segid "BrD " and resid 106  and name HN  ))
    4 900     4 900     0 600 peak 14001 weight  0 10000E+01 volume  0 12922E+02 ppm1      8 529 ppm2      9 745
ASSI {14021}
  (( segid "BrD " and resid 108  and name HN  ))
  (( segid "BrD " and resid 104  and name HA  ))
    2 700     1 800     1 800 peak 14021 weight  0 10000E+01 volume  0.54819E+03 ppm1      8 526 ppm2      4 663
ASSI {14031}
  (( segid "BrD " and resid 108  and name HN  ))
  (( segid "BrD " and resid 110  and name HG12))
    5 200     5 200     0.300 peak 14031 weight  0 10000E+01 volume  0 95149E+01 ppm1      8.521 ppm2      1 696
ASSI {14051}
  (( segid "BrD " and resid 107  and name HN  ))
  (( segid "BrD " and resid 108  and name HA  ))
    4 500     4 500     1 000 peak 14051 weight  0 10000E+01 volume  0 23253E+02 ppm1      8.980 ppm2      4 798
ASSI {14081}
  (( segid "BrD " and resid 106  and name HN  ))
  (  segid "BrD " and resid 21   and name HG2%)
    4 600     4 600     0 900 peak 14081 weight  0 10000E+01 volume  0 21267E+02 ppm1      9 740 ppm2      1 640
ASSI {14091}
  (( segid "BrD " and resid 105  and name HN  ))
  (( segid "BrD " and resid 106  and name HA  ))
    4 500     4 500     1 000 peak 14091 weight  0 10000E+01 volume  0 22190E+02 ppm1      8 487 ppm2      4 568
ASSI {14101}
  (( segid "BrD " and resid 105  and name HN  ))
  (( segid "BrD " and resid 103  and name HB2 ))
    5 000     5 000     0.500 peak 14101 weight  0 10000E+01 volume  0 11917E+02 ppm1      8 487 ppm2      1 881
ASSI {14181}
  (( segid "BrD " and resid 100  and name HN  ))
  (( segid "BrD " and resid 34   and name HZ  ))
    4 700     4 700     0.800 peak 14181 weight  0 10000E+01 volume  0 18067E+02 ppm1      8 675 ppm2      7.907
ASSI {14211}
  (( segid "BrD " and resid 100  and name HN  ))
  (( segid "BrD " and resid 97   and name HB1 ))
    4 400     4 400     1 100 peak 14211 weight  0 10000E+01 volume  0 25437E+02 ppm1      8 669 ppm2      2 715
ASSI {14231}
  (( segid "BrD " and resid 99   and name HN  ))
  (( segid "BrD " and resid 101  and name HN  ))
    4 300     4 300     1.200 peak 14231 weight  0 10000E+01 volume  0 28380E+02 ppm1      8 936 ppm2      8 500
ASSI {14261}
  (( segid "BrD " and resid 99   and name HN  ))
  (( segid "BrD " and resid 33   and name HG1 ))
    5 500     5.500     0 000 peak 14261 weight  0.10000E+01 volume  0 32802E+01 ppm1      8 936 ppm2      0 866
ASSI {14271}
  (( segid "BrD " and resid 98   and name HN  ))
  (( segid "BrD " and resid 101  and name HN  ))
    4 400     4.400     1 100 peak 14271 weight  0.10000E+01 volume  0 25780E+02 ppm1      9 125 ppm2      8 515
ASSI {14291}
  (( segid "BrD " and resid 97   and name HN  ))
  (( segid "BrD " and resid 93   and name HB1 ))
    5 500     5 500     0.000 peak 14291 weight  0 10000E+01 volume  0 62831E+01 ppm1      8 677 ppm2      5 016
OR {14291}
  (( segid "BrD " and resid 97   and name HN  ))
  (( segid "BrD " and resid 93   and name HA  ))
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ASSI {14321}
  (( segid "BrD " and resid 95    and name HN  ))
  (( segid "BrD " and resid 32    and name HH2 ))
   3 700     3 400      1 800 peak 14321 weight  0 10000E+01 volume  0 76926E+02 ppm1    8 669 ppm2    7 739
ASSI {14331}
  (( segid "BrD " and resid 93    and name HN  ))
  (( segid "BrD " and resid 96    and name HN  ))
   4 500     4 500      1.000 peak 14331 weight  0 10000E+01 volume  0 22598E+02 ppm1    8.713 ppm2    7 963
ASSI {14351}
  (( segid "BrD " and resid 93    and name HN  ))
  (( segid "BrD " and resid 95    and name HB1 ))
   4 600     4 600      0.900 peak 14351 weight  0.10000E+01 volume  0 20643E+02 ppm1    8.714 ppm2    3 617
ASSI {14381}
  (( segid "BrD " and resid 87    and name HN  ))
  (( segid "BrD " and resid 89    and name HD21))
   3 900     3.800      1 600 peak 14381 weight  0 10000E+01 volume  0 54969E+02 ppm1    8 568 ppm2    8 959
ASSI {14391}
  (( segid "BrD " and resid 87    and name HN  ))
  (( segid "BrD " and resid 89    and name HN  ))
   3 600     3 200      1 900 peak 14391 weight  0.10000E+01 volume  0 81305E+02 ppm1    8 568 ppm2    8 838
ASSI {14431}
  (( segid "BrD " and resid 85    and name HN  ))
  (( segid "BrD " and resid 87    and name HN  ))
   4 100     4 100      1.400 peak 14431 weight  0 10000E+01 volume  0 42435E+02 ppm1    7 516 ppm2    8 557
ASSI {14471}
  (( segid "BrD " and resid 82    and name HN  ))
  (( segid "BrD " and resid 80    and name HN  ))
   4 800     4 800      0.700 peak 14471 weight  0 10000E+01 volume  0 16164E+02 ppm1    6 979 ppm2    7 979
ASSI {14521}
  (( segid "BrD " and resid 79    and name HN  ))
  (( segid "BrD " and resid 77    and name HA  ))
   4 800     4 800      0 700 peak 14521 weight  0 10000E+01 volume  0 15931E+02 ppm1    8 679 ppm2    4 968
ASSI {14531}
  (( segid "BrD " and resid 79    and name HN  ))
  (  segid "BrD " and resid 59    and name HE% )
   4 000     4 000      1 500 peak 14531 weight  0 10000E+01 volume  0 45701E+02 ppm1    8 680 ppm2    1 876
ASSI {14561}
  (( segid "BrD " and resid 76    and name HN  ))
  (( segid "BrD " and resid 74    and name HA  ))
   4 300     4 300      1 200 peak 14561 weight  0 10000E+01 volume  0 31541E+02 ppm1    8 611 ppm2    4 361
ASSI {14601}
  (( segid "BrD " and resid 72    and name HN  ))
  (( segid "BrD " and resid 75    and name HB2 ))
   4 600     4 600      0 900 peak 14601 weight  0 10000E+01 volume  0 21235E+02 ppm1    8 859 ppm2    2 805
ASSI {14611}
  (( segid "BrD " and resid 72    and name HN  ))
  (( segid "BrD " and resid 9     and name HB1 ))
   3 600     3 200      1 900 peak 14611 weight  0 10000E+01 volume  0 90159E+02 ppm1    8 859 ppm2    2 443
ASSI {14661}
  (( segid "BrD " and resid 64    and name HN  ))
  (( segid "BrD " and resid 62    and name HN  ))
   4 100     4 100      1 400 peak 14661 weight  0 10000E+01 volume  0 40125E+02 ppm1    8 585 ppm2    8 966
ASSI {14681}
  (( segid "BrD " and resid 64    and name HN  ))
  (( segid "BrD " and resid 65    and name HB2 ))
   4 800     4 800      0 700 peak 14681 weight  0 10000E+01 volume  0 16509E+02 ppm1    8 584 ppm2    3 383
ASSI {14711}
  (( segid "BrD " and resid 63    and name HN  ))
  (  segid "BrD " and resid 74    and name HD% )
   4 600     4 600      0 900 peak 14711 weight  0 10000E+01 volume  0 18909E+02 ppm1    9 471 ppm2    7 007
ASSI {14741}
  (( segid "BrD " and resid 62    and name HN  ))
  (( segid "BrD " and resid 61    and name HN  ))
   2 600     1 700      1 700 peak 14741 weight  0 10000E+01 volume  0 63142E+03 ppm1    8 997 ppm2    8 742
ASSI {14771}
  (( segid "BrD " and resid 62    and name HN  ))
  (( segid "BrD " and resid 65    and name HB2 ))
   4 200     4 200      1 300 peak 14771 weight  0 10000E+01 volume  0 33744E+02 ppm1    8 999 ppm2    3 355
ASSI {14841}
  (( segid "BrD " and resid 57    and name HN  ))
  (( segid "BrD " and resid 35    and name HA  ))
   3 200     2.600      2 300 peak 14841 weight  0 10000E+01 volume  0 16187E+03 ppm1    9 359 ppm2    4 904
ASSI {14861}
  (( segid "BrD " and resid 55    and name HN  ))
  (( segid "BrD " and resid 59    and name HN  ))
   3 900     3 800      1 600 peak 14861 weight  0 10000E+01 volume  0 53302E+02 ppm1    7 974 ppm2    8 498
ASSI {14891}
  (( segid "BrD " and resid 54    and name HN  ))
  (( segid "BrD " and resid 84    and name HB1 ))
   4 600     4 600      0.900 peak 14891 weight  0 10000E+01 volume  0 21172E+02 ppm1    9 037 ppm2    3 597
ASSI {14981}
  (( segid "BrD " and resid 48    and name HN  ))
  (( segid "BrD " and resid 46    and name HB2 ))
   4 300     4 300      1 200 peak 14981 weight  0 10000E+01 volume  0 30250E+02 ppm1    8.306 ppm2    3 090
ASSI {14991}
  (( segid "BrD " and resid 48    and name HN  ))
  (  segid "BrD " and resid 49    and name HG1%)
   3 700     3 400      1 800 peak 14991 weight  0 10000E+01 volume  0 71559E+02 ppm1    8.305 ppm2    1 639
ASSI {15001}
  (( segid "BrD " and resid 92    and name HN  ))
  (( segid "BrD " and resid 89    and name HD22))
   4.900     4 900      0.600 peak 15001 weight  0 10000E+01 volume  0 14588E+02 ppm1    8 832 ppm2    8 433
ASSI {15011}
  (( segid "BrD " and resid 47    and name HN  ))
  (( segid "BrD " and resid 49    and name HN  ))
   4 000     4 000      1 500 peak 15011 weight  0 10000E+01 volume  0 44203E+02 ppm1    8 832 ppm2    7 759
ASSI {15041}
  (( segid "BrD " and resid 43    and name HN  ))
  (( segid "BrD " and resid 42    and name HG1 ))
   4 000     4 000      1 500 peak 15041 weight  0 10000E+01 volume  0 44922E+02 ppm1    8 000 ppm2    2 889
ASSI {15071}
  (( segid "BrD " and resid 35    and name HN  ))
  (( segid "BrD " and resid 33    and name HA  ))
   4 300     4 300      1 200 peak 15071 weight  0 10000E+01 volume  0 32086E+02 ppm1    7 735 ppm2    4 346
ASSI {15081}
  (( segid "BrD " and resid 35    and name HN  ))
  (( segid "BrD " and resid 34    and name HB1 ))
   3.800     3 600      1 700 peak 15081 weight  0 10000E+01 volume  0 61308E+02 ppm1    7 734 ppm2    4 079
ASSI {15111}
  (( segid "BrD " and resid 34    and name HN  ))
  (  segid "BrD " and resid 81    and name HG2%)
   4 700     4 700      0.800 peak 15111 weight  0 10000E+01 volume  0 17971E+02 ppm1    8 178 ppm2    0 756
ASSI {15131}
  (( segid "BrD " and resid 32    and name HN  ))
  (( segid "BrD " and resid 33    and name HG1 ))
   5 400     5 400      0 100 peak 15131 weight  0 10000E+01 volume  0 80093E+01 ppm1    7 739 ppm2    0 859
ASSI {15141}
  (( segid "BrD " and resid 31    and name HN  ))
  (( segid "BrD " and resid 28    and name HN  ))
   3 200     2 600      2 300 peak 15141 weight  0 10000E+01 volume  0 16166E+03 ppm1    8 480 ppm2    8 159
OR {15141}
  (( segid "BrD " and resid 31    and name HN  ))
  (( segid "BrD " and resid 28    and name HE1 ))
ASSI {15161}
  (( segid "BrD " and resid 30    and name HN  ))
  (  segid "BrD " and resid 31    and name HB% )
   3 800     3 600      1 700 peak 15161 weight  0 10000E+01 volume  0 65201E+02 ppm1    12 276 ppm2   2 299
ASSI {15171}
  (( segid "BrD " and resid 30    and name HN  ))
  (  segid "BrD " and resid 102   and name HD1%)
   3 900     3 800      1 600 peak 15171 weight  0 10000E+01 volume  0 51602E+02 ppm1    12 275 ppm2   1 315
ASSI {15191}
  (( segid "BrD " and resid 29    and name HN  ))
  (( segid "BrD " and resid 31    and name HN  ))
   5 000     5 000      0 500 peak 15191 weight  0.10000E+01 volume  0 12673E+02 ppm1    9 152 ppm2    8 470
ASSI {15201}
  (( segid "BrD " and resid 29    and name HN  ))
  (( segid "BrD " and resid 30    and name HB1 ))
   4 300     4 300      1 200 peak 15201 weight  0.10000E+01 volume  0 29023E+02 ppm1    9 151 ppm2    4 941
ASSI {15211}
  (( segid "BrD " and resid 29    and name HN  ))
  (  segid "BrD " and resid 101   and name HD1%)
   5 000     5 000      0 500 peak 15211 weight  0 10000E+01 volume  0 12825E+02 ppm1    9 153 ppm2    1 558
ASSI {15261}
  (( segid "BrD " and resid 27    and name HN  ))
  (( segid "BrD " and resid 28    and name HB1 ))
   4 400     4 400      1 100 peak 15261 weight  0 10000E+01 volume  0 27022E+02 ppm1    8.169 ppm2    3 575
ASSI {15291}
  (( segid "BrD " and resid 26    and name HN  ))
  (( segid "BrD " and resid 24    and name HN  ))
   3 500     3 100      2.000 peak 15291 weight  0 10000E+01 volume  0 10602E+03 ppm1    9 196 ppm2    8 655
ASSI {15311}
  (( segid "BrD " and resid 25    and name HN  ))
  (( segid "BrD " and resid 24    and name HE22))
   4 900     4 900      0 600 peak 15311 weight  0.10000E+01 volume  0 14311E+02 ppm1    9 133 ppm2    7 489
ASSI {15361}
  (( segid "BrD " and resid 24    and name HN  ))
  (( segid "BrD " and resid 24    and name HE21))
   4 000     4 000      1 500 peak 15361 weight  0 10000E+01 volume  0 49074E+02 ppm1    8 659 ppm2    7.616
ASSI {15381}
  (( segid "BrD " and resid 19    and name HN  ))
  (  segid "BrD " and resid 75    and name HE% )
   5 500     5 500      0 000 peak 15381 weight  0 10000E+01 volume  0 38565E-01 ppm1    9 187 ppm2    2 654
ASSI {15391}
  (( segid "BrD " and resid 19    and name HN  ))
  (( segid "BrD " and resid 63    and name HG  ))
   4 500     4 500      1 000 peak 15391 weight  0 10000E+01 volume  0 24115E+02 ppm1    9 188 ppm2    2 454
ASSI {15401}
  (( segid "BrD " and resid 18    and name HN  ))
  (( segid "BrD " and resid 21    and name HN  ))
   3 900     3 800      1 600 peak 15401 weight  0 10000E+01 volume  0 53379E+02 ppm1    9 072 ppm2    8 558
ASSI {15421}
  (( segid "BrD " and resid 17    and name HN  ))
  (( segid "BrD " and resid 16    and name HN  ))
   2.800     2 000      2 000 peak 15421 weight  0 10000E+01 volume  0 36762E+03 ppm1    8 669 ppm2    8 780
ASSI {15441}
  (( segid "BrD " and resid 17    and name HN  ))
  (( segid "BrD " and resid 20    and name HN  ))
   3 500     3.100      2 000 peak 15441 weight  0.10000E+01 volume  0.95968E+02 ppm1    8 668 ppm2    8 154
ASSI {15481}
  (( segid "BrD " and resid 15    and name HN  ))
  (  segid "BrD " and resid 18    and name HD1%)
   5.500     5 500      0 000 peak 15481 weight  0.10000E+01 volume  0.62753E+01 ppm1    8 599 ppm2    1.069
ASSI {15511}
  (( segid "BrD " and resid 12    and name HN  ))
  (( segid "BrD " and resid 10    and name HA  ))
   3 900     3 800      1 600 peak 15511 weight  0 10000E+01 volume  0 54637E+02 ppm1    9 023 ppm2    5 464
ASSI {15531}
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(( segid "BrD " and resid 10   and name HN  ))
(( segid "BrD " and resid 8    and name HD2 ))
   5 200     5 200     0 300 peak 15531 weight  0 10000E+01 volume  0 99597E+01 ppm1      8 885 ppm2      4.288
ASSI {15551}
 (( segid "BrD " and resid 7    and name HN  ))
 (( segid "BrD " and resid 8    and name HD2 ))
   4 900     4 900     0 600 peak 15551 weight  0.10000E+01 volume  0 14339E+02 ppm1      8 924 ppm2      4 281
ASSI {15631}
 (( segid "BrD " and resid 32   and name HE1 ))
 (( segid "BrD " and resid 33   and name HD2 ))
   3 800     3 600     1 700 peak 15631 weight  0.10000E+01 volume  0 61547E+02 ppm1     11 082 ppm2      2 167
ASSI {15641}
 (( segid "BrD " and resid 67   and name HN  ))
 (( segid "BrD " and resid 62   and name HA  ))
   4 600     4.600     0 900 peak 15641 weight  0 10000E+01 volume  0 20420E+02 ppm1      8 632 ppm2      4 471
ASSI {27052}
 (( segid "BrD " and resid 89   and name HB1 ))
 (( segid "BrD " and resid 91   and name HD1 ))
   3 600     3 200     1 900 peak 27052 weight  0 11000E+01 volume  0 39185E+02 ppm1      3 669 ppm2      4 556
ASSI {27062}
 (( segid "BrD " and resid 89   and name HB2 ))
 (( segid "BrD " and resid 91   and name HD1 ))
   3 700     3 400     1 800 peak 27062 weight  0 11000E+01 volume  0 32055E+02 ppm1      3 473 ppm2      4 556
ASSI {27072}
 (( segid "BrD " and resid 89   and name HB2 ))
 (( segid "BrD " and resid 91   and name HD2 ))
   3 400     2 900     2 100 peak 27072 weight  0 11000E+01 volume  0 54263E+02 ppm1      3 473 ppm2      4 411
ASSI {26992}
 (( segid "BrD " and resid 89   and name HA  ))
 (( segid "BrD " and resid 91   and name HG1 ))
   3 400     2 900     2 100 peak 26992 weight  0 11000E+01 volume  0 54091E+02 ppm1      5 642 ppm2      2 792
OR {26992}
 (( segid "BrD " and resid 89   and name HA  ))
 (( segid "BrD " and resid 91   and name HG2 ))
ASSI {26732}
 (( segid "BrD " and resid 94   and name HG1 ))
 (  segid "BrD " and resid 95   and name HD% )
   3 300     2 700     2 200 peak 26732 weight  0 11000E+01 volume  0 57563E+02 ppm1      3 127 ppm2      7 505
OR {26732}
 (( segid "BrD " and resid 94   and name HG2 ))
 (  segid "BrD " and resid 95   and name HD% )
ASSI {26822}
 (( segid "BrD " and resid 94   and name HB2 ))
 (  segid "BrD " and resid 95   and name HD% )
   3 000     2 200     2.200 peak 26822 weight  0 11000E+01 volume  0 10961E+03 ppm1      2 733 ppm2      7 506
OR {26822}
 (( segid "BrD " and resid 94   and name HB1 ))
 (  segid "BrD " and resid 95   and name HD% )
ASSI {19122}
 (  segid "BrD " and resid 43   and name HB% )
 (  segid "BrD " and resid 47   and name HE% )
   3 900     3 800     1.600 peak 19122 weight  0 11000E+01 volume  0 23047E+02 ppm1      1 697 ppm2      7 267
ASSI {    2}
 (( segid "BrD " and resid 93   and name HA  ))
 (( segid "BrD " and resid 93   and name HB2 ))
   2 100     1 100     1 100 peak     2 weight  0 11000E+01 volume  0 10291E+04 ppm1      5 003 ppm2      4 766
ASSI {   22}
 (( segid "BrD " and resid 108  and name HB1 ))
 (( segid "BrD " and resid 108  and name HA  ))
   1 800     0 800     0 800 peak    22 weight  0 11000E+01 volume  0 21120E+04 ppm1      4 603 ppm2      4 801
ASSI {   32}
 (( segid "BrD " and resid 70   and name HA  ))
 (( segid "BrD " and resid 70   and name HB1 ))
   2 500     1 600     1 600 peak    32 weight  0 11000E+01 volume  0 29221E+03 ppm1      5 344 ppm2      4 786
ASSI {   62}
 (( segid "BrD " and resid 70   and name HB2 ))
 (( segid "BrD " and resid 70   and name HA  ))
   2 500     1 600     1 600 peak    62 weight  0 11000E+01 volume  0 30042E+03 ppm1      4 360 ppm2      5 360
ASSI {   72}
 (( segid "BrD " and resid 20   and name HA  ))
 (( segid "BrD " and resid 20   and name HB1 ))
   2 100     1 100     1 100 peak    72 weight  0 11000E+01 volume  0 10650E+04 ppm1      4 901 ppm2      4 670
ASSI {   92}
 (( segid "BrD " and resid 27   and name HA  ))
 (( segid "BrD " and resid 27   and name HB1 ))
   2 100     1.100     1 100 peak    92 weight  0 11000E+01 volume  0 83585E+03 ppm1      5 050 ppm2      4 617
ASSI {  112}
 (( segid "BrD " and resid 38   and name HA  ))
 (  segid "BrD " and resid 38   and name HG2%)
   2 600     1 700     1 700 peak   112 weight  0 11000E+01 volume  0 24356E+03 ppm1      4 162 ppm2      0 792
ASSI {  132}
 (( segid "BrD " and resid 38   and name HB  ))
 (  segid "BrD " and resid 38   and name HG1%)
   2 400     1 400     1 400 peak   132 weight  0 11000E+01 volume  0.41156E+03 ppm1      1 751 ppm2      1 076
ASSI {  152}
 (  segid "BrD " and resid 38   and name HG2%)
 (( segid "BrD " and resid 38   and name HB  ))
   2 300     1 300     1 300 peak   152 weight  0.11000E+01 volume  0 59973E+03 ppm1      0 808 ppm2      1 776
ASSI {  232}
 (( segid "BrD " and resid 81   and name HB  ))
 (  segid "BrD " and resid 81   and name HG1%)
   2 400     1.400     1 400 peak   232 weight  0 11000E+01 volume  0.37056E+03 ppm1      2 042 ppm2      1 079
ASSI {  242}
 (( segid "BrD " and resid 81   and name HB  ))
 (  segid "BrD " and resid 81   and name HG2%)
   2 300     1 300     1 300 peak   242 weight  0.11000E+01 volume  0.47548E+03 ppm1      2 042 ppm2      0 759
ASSI {  262}
 (( segid "BrD " and resid 15   and name HA  ))
 (( segid "BrD " and resid 15   and name HB1 ))
   2 700     1 800     1.800 peak   262 weight  0 11000E+01 volume  0 20830E+03 ppm1      4.607 ppm2      3 811
ASSI {  322}
 (( segid "BrD " and resid 46   and name HB1 ))
 (( segid "BrD " and resid 46   and name HA  ))
   2 700     1 800     1 800 peak   322 weight  0 11000E+01 volume  0 21305E+03 ppm1      3 274 ppm2      4 143
ASSI {  332}
 (( segid "BrD " and resid 46   and name HB2 ))
 (( segid "BrD " and resid 46   and name HA  ))
   2 700     1 800     1 800 peak   332 weight  0.11000E+01 volume  0 21514E+03 ppm1      3 077 ppm2      4 143
ASSI {  352}
 (( segid "BrD " and resid 47   and name HA  ))
 (( segid "BrD " and resid 47   and name HB2 ))
   2.700     1.800     1 800 peak   352 weight  0 11000E+01 volume  0 22249E+03 ppm1      4 704 ppm2      3 395
ASSI {  362}
 (( segid "BrD " and resid 47   and name HB1 ))
 (( segid "BrD " and resid 47   and name HA  ))
   2 600     1 700     1.700 peak   362 weight  0 11000E+01 volume  0 23254E+03 ppm1      3 815 ppm2      4 721
ASSI {  382}
 (( segid "BrD " and resid 67   and name HA  ))
 (( segid "BrD " and resid 67   and name HB1 ))
   2 400     1.400     1 400 peak   382 weight  0 11000E+01 volume  0 45818E+03 ppm1      4 654 ppm2      3 572
ASSI {  392}
 (( segid "BrD " and resid 67   and name HA  ))
 (( segid "BrD " and resid 67   and name HB2 ))
   2 500     1 600     1 600 peak   392 weight  0.11000E+01 volume  0 31584E+03 ppm1      4 653 ppm2      2 669
ASSI {  422}
 (( segid "BrD " and resid 68   and name HB1 ))
 (( segid "BrD " and resid 68   and name HA  ))
   3 100     2 400     2 400 peak   422 weight  0.11000E+01 volume  0 94493E+02 ppm1      3.669 ppm2      5 143
ASSI {  432}
 (( segid "BrD " and resid 68   and name HB2 ))
 (( segid "BrD " and resid 68   and name HA  ))
   2 700     1 800     1 800 peak   432 weight  0 11000E+01 volume  0 18471E+03 ppm1      3 522 ppm2      5 143
ASSI {  472}
 (( segid "BrD " and resid 88   and name HB1 ))
 (( segid "BrD " and resid 88   and name HA  ))
   2 600     1 700     1 700 peak   472 weight  0 11000E+01 volume  0 28741E+03 ppm1      3 522 ppm2      4 989
ASSI {  492}
 (( segid "BrD " and resid 95   and name HA  ))
 (( segid "BrD " and resid 95   and name HB2 ))
   2 600     1 700     1 700 peak   492 weight  0 11000E+01 volume  0 23932E+03 ppm1      4 459 ppm2      3 361
ASSI {  502}
 (( segid "BrD " and resid 95   and name HB1 ))
 (( segid "BrD " and resid 95   and name HA  ))
   2 600     1 700     1 700 peak   502 weight  0 11000E+01 volume  0 28555E+03 ppm1      3 619 ppm2      4 444
ASSI {  522}
 (( segid "BrD " and resid 96   and name HA  ))
 (( segid "BrD " and resid 96   and name HB1 ))
   2 800     2 000     2 000 peak   522 weight  0 11000E+01 volume  0 17185E+03 ppm1      4 409 ppm2      3 998
ASSI {  532}
 (( segid "BrD " and resid 96   and name HA  ))
 (( segid "BrD " and resid 96   and name HD2 ))
   2 800     2 000     2 000 peak   532 weight  0.11000E+01 volume  0 16898E+03 ppm1      4 409 ppm2      3 118
ASSI {  562}
 (( segid "BrD " and resid 31   and name HA  ))
 (  segid "BrD " and resid 31   and name HB% )
   2 500     1 600     1 600 peak   562 weight  0 11000E+01 volume  0 36354E+03 ppm1      5 000 ppm2      2 315
ASSI {  592}
 (  segid "BrD " and resid 43   and name HB% )
 (( segid "BrD " and resid 43   and name HA  ))
   2 200     1 200     1 200 peak   592 weight  0 11000E+01 volume  0 76123E+03 ppm1      1 700 ppm2      5 539
ASSI {  612}
 (  segid "BrD " and resid 76   and name HB% )
 (( segid "BrD " and resid 76   and name HA  ))
   2 100     1 100     1 100 peak   612 weight  0.11000E+01 volume  0 87848E+03 ppm1      2 093 ppm2      4 687
ASSI {  632}
 (  segid "BrD " and resid 99   and name HB% )
 (( segid "BrD " and resid 99   and name HA  ))
   2 000     1 000     1 000 peak   632 weight  0.11000E+01 volume  0 10742E+04 ppm1      2 190 ppm2      4 440
ASSI {  642}
 (( segid "BrD " and resid 113  and name HA  ))
 (  segid "BrD " and resid 113  and name HB% )
   2.100     1 100     1 100 peak   642 weight  0 11000E+01 volume  0 84264E+03 ppm1      4.901 ppm2      1 979
ASSI {  662}
 (( segid "BrD " and resid 34   and name HA  ))
 (( segid "BrD " and resid 34   and name HB1 ))
   2 600     1 700     1 700 peak   662 weight  0.11000E+01 volume  0 27701E+03 ppm1      5 542 ppm2      4 107
ASSI {  672}
 (( segid "BrD " and resid 34   and name HA  ))
 (( segid "BrD " and resid 34   and name HB2 ))
   2.800     2 000     2.000 peak   672 weight  0 11000E+01 volume  0 16922E+03 ppm1      5 542 ppm2      3 146
ASSI {  702}
 (( segid "BrD " and resid 74   and name HA  ))
 (( segid "BrD " and resid 74   and name HB1 ))
   3 000     2 200     2 200 peak   702 weight  0 11000E+01 volume  0 10996E+03 ppm1      4.359 ppm2      3 563
ASSI {  712}
 (( segid "BrD " and resid 74   and name HA  ))
 (( segid "BrD " and resid 74   and name HB2 ))
   3 100     2 400     2 400 peak   712 weight  0 11000E+01 volume  0 88126E+02 ppm1      4 361 ppm2      3 000
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ASSI {  742}
   (( segid "BrD " and resid 82   and name HA  ))
   (( segid "BrD " and resid 82   and name HB1 ))
     2 800     2 000     2.000 peak   742 weight  0 11000E+01 volume  0 15835E+03 ppm1      4 755 ppm2     3 695
ASSI {  752}
   (( segid "BrD " and resid 82   and name HA  ))
   (( segid "BrD " and resid 82   and name HB2 ))
     2.700     1 800     1 800 peak   752 weight  0.11000E+01 volume  0 18532E+03 ppm1      4 755 ppm2     3 573
ASSI {  792}
   (( segid "BrD " and resid 106  and name HA  ))
   (( segid "BrD " and resid 106  and name HB1 ))
     2 700     1 800     1 800 peak   792 weight  0.11000E+01 volume  0 19130E+03 ppm1      4.558 ppm2     3 916
ASSI {  802}
   (( segid "BrD " and resid 106  and name HA  ))
   (( segid "BrD " and resid 106  and name HB2 ))
     2 600     1 700     1 700 peak   802 weight  0 11000E+01 volume  0 25966E+03 ppm1      4 557 ppm2     3.702
ASSI {  842}
   (( segid "BrD " and resid 107  and name HB1 ))
   (( segid "BrD " and resid 107  and name HA  ))
     2 200     1 200     1 200 peak   842 weight  0 11000E+01 volume  0 64742E+03 ppm1      3 671 ppm2     4 435
ASSI {  872}
   (( segid "BrD " and resid 65   and name HA  ))
   (( segid "BrD " and resid 65   and name HB1 ))
     2 600     1 700     1 700 peak   872 weight  0 11000E+01 volume  0 23368E+03 ppm1      5 398 ppm2     3 621
ASSI {  882}
   (( segid "BrD " and resid 65   and name HA  ))
   (( segid "BrD " and resid 65   and name HB2 ))
     2 900     2 100     2.100 peak   882 weight  0.11000E+01 volume  0.14380E+03 ppm1      5 396 ppm2     3 369
ASSI {  892}
   (( segid "BrD " and resid 84   and name HA  ))
   (( segid "BrD " and resid 84   and name HB1 ))
     2.700     1 800     1 800 peak   892 weight  0 11000E+01 volume  0.20950E+03 ppm1      4 904 ppm2     3 606
ASSI {  902}
   (( segid "BrD " and resid 84   and name HA  ))
   (( segid "BrD " and resid 84   and name HB2 ))
     2 600     1 700     1 700 peak   902 weight  0 11000E+01 volume  0 23639E+03 ppm1      4 904 ppm2     3 272
ASSI {  942}
   (( segid "BrD " and resid 100  and name HB2 ))
   (( segid "BrD " and resid 100  and name HA  ))
     2 300     1 300     1 300 peak   942 weight  0 11000E+01 volume  0 53744E+03 ppm1      3 424 ppm2     4 949
ASSI {  952}
   (( segid "BrD " and resid 10   and name HA  ))
   (( segid "BrD " and resid 10   and name HB1 ))
     3 200     2 600     2 300 peak   952 weight  0 11000E+01 volume  0 81254E+02 ppm1      5 478 ppm2     3 354
ASSI {  972}
   (( segid "BrD " and resid 12   and name HA  ))
   (( segid "BrD " and resid 12   and name HB1 ))
     2 700     1 800     1 800 peak   972 weight  0 11000E+01 volume  0 22766E+03 ppm1      5 297 ppm2     3 434
ASSI {  992}
   (( segid "BrD " and resid 77   and name HA  ))
   (( segid "BrD " and resid 77   and name HB1 ))
     2 500     1 600     1.600 peak   992 weight  0 11000E+01 volume  0 33274E+03 ppm1      4 951 ppm2     3 319
ASSI { 1032}
   (( segid "BrD " and resid 117  and name HB2 ))
   (( segid "BrD " and resid 117  and name HA  ))
     2 700     1 800     1 800 peak  1032 weight  0 11000E+01 volume  0 21830E+03 ppm1      3 127 ppm2     5.167
ASSI { 1042}
   (( segid "BrD " and resid 117  and name HB1 ))
   (( segid "BrD " and resid 117  and name HA  ))
     2 600     1 700     1 700 peak  1042 weight  0 11000E+01 volume  0 23430E+03 ppm1      3 301 ppm2     5 167
ASSI { 1052}
   (( segid "BrD " and resid 89   and name HA  ))
   (( segid "BrD " and resid 89   and name HB1 ))
     2.900     2 100     2 100 peak  1052 weight  0 11000E+01 volume  0.12958E+03 ppm1      5 641 ppm2     3 668
ASSI { 1062}
   (( segid "BrD " and resid 89   and name HA  ))
   (( segid "BrD " and resid 89   and name HB2 ))
     2 800     2 000     2 000 peak  1062 weight  0 11000E+01 volume  0 16727E+03 ppm1      5 641 ppm2     3 491
ASSI { 1092}
   (( segid "BrD " and resid 18   and name HA  ))
   (( segid "BrD " and resid 18   and name HG  ))
     3 100     2 400     2 400 peak  1092 weight  0 11000E+01 volume  0 85824E+02 ppm1      3 866 ppm2     2 277
ASSI { 1132}
   (  segid "BrD " and resid 18   and name HD2%)
   (( segid "BrD " and resid 18   and name HA  ))
     2 100     1 100     1 100 peak  1132 weight  0 11000E+01 volume  0 86347E+03 ppm1      0 415 ppm2     3 883
ASSI { 1142}
   (  segid "BrD " and resid 18   and name HD2%)
   (( segid "BrD " and resid 18   and name HG  ))
     2.500     1 600     1 600 peak  1142 weight  0 11000E+01 volume  0.31482E+03 ppm1      0 419 ppm2     2 274
ASSI { 1162}
   (( segid "BrD " and resid 78   and name HA  ))
   (( segid "BrD " and resid 78   and name HB2 ))
     2 500     1.600     1.600 peak  1162 weight  0.11000E+01 volume  0.33654E+03 ppm1      3 968 ppm2     1 044
ASSI { 1172}
   (( segid "BrD " and resid 78   and name HA  ))
   (( segid "BrD " and resid 78   and name HG  ))
     2 900     2 100     2 100 peak  1172 weight  0 11000E+01 volume  0 14454E+03 ppm1      3 967 ppm2     1 270
ASSI { 1202}
   (( segid "BrD " and resid 78   and name HB1 ))
   (( segid "BrD " and resid 78   and name HA  ))
     2 700     1.800     1.800 peak  1202 weight  0 11000E+01 volume  0 21843E+03 ppm1      1.305 ppm2     4 001
ASSI { 1212}
   (( segid "BrD " and resid 78   and name HB1 ))
   (  segid "BrD " and resid 78   and name HD1%)
     2 900     2 100     2 100 peak  1212 weight  0 11000E+01 volume  0 13310E+03 ppm1      1 305 ppm2     0 776
ASSI { 1222}
   (( segid "BrD " and resid 78   and name HB1 ))
   (  segid "BrD " and resid 78   and name HD2%)
     2 700     1 800     1 800 peak  1222 weight  0 11000E+01 volume  0.22009E+03 ppm1      1 305 ppm2     0 673
ASSI { 1262}
   (( segid "BrD " and resid 78   and name HG  ))
   (( segid "BrD " and resid 78   and name HB2 ))
     2.400     1 400     1 400 peak  1262 weight  0 11000E+01 volume  0 41554E+03 ppm1      1 254 ppm2     1 043
ASSI { 1282}
   (  segid "BrD " and resid 78   and name HD1%)
   (( segid "BrD " and resid 78   and name HA  ))
     2 400     1 400     1 400 peak  1282 weight  0 11000E+01 volume  0 38399E+03 ppm1      0 761 ppm2     3 998
ASSI { 1302}
   (  segid "BrD " and resid 78   and name HD1%)
   (( segid "BrD " and resid 78   and name HB2 ))
     2 600     1 700     1 700 peak  1302 weight  0 11000E+01 volume  0.25846E+03 ppm1      0 761 ppm2     1 038
ASSI { 1312}
   (  segid "BrD " and resid 78   and name HD1%)
   (( segid "BrD " and resid 78   and name HG  ))
     2 200     1 200     1 200 peak  1312 weight  0 11000E+01 volume  0 70030E+03 ppm1      0 761 ppm2     1 270
ASSI { 1322}
   (( segid "BrD " and resid 115  and name HA  ))
   (( segid "BrD " and resid 115  and name HB1 ))
     2.200     1 200     1 200 peak  1322 weight  0 11000E+01 volume  0 70481E+03 ppm1      4 807 ppm2     2 182
ASSI { 1352}
   (  segid "BrD " and resid 115  and name HD1%)
   (( segid "BrD " and resid 115  and name HA  ))
     3.300     2 700     2 200 peak  1352 weight  0 11000E+01 volume  0 57522E+02 ppm1      1 352 ppm2     4 829
ASSI { 1362}
   (  segid "BrD " and resid 115  and name HD1%)
   (( segid "BrD " and resid 115  and name HG  ))
     2 400     1 400     1 400 peak  1362 weight  0.11000E+01 volume  0 44618E+03 ppm1      1 352 ppm2     2 148
ASSI { 1382}
   (( segid "BrD " and resid 116  and name HB  ))
   (( segid "BrD " and resid 116  and name HA  ))
     2.700     1 800     1 800 peak  1382 weight  0 11000E+01 volume  0 19754E+03 ppm1      2 411 ppm2     4 823
ASSI { 1402}
   (( segid "BrD " and resid 116  and name HB  ))
   (( segid "BrD " and resid 116  and name HG12))
     2.200     1 200     1 200 peak  1402 weight  0 11000E+01 volume  0 69385E+03 ppm1      2 409 ppm2     1 555
ASSI { 1422}
   (( segid "BrD " and resid 116  and name HG11))
   (( segid "BrD " and resid 116  and name HB  ))
     2.500     1 600     1.600 peak  1422 weight  0 11000E+01 volume  0 30727E+03 ppm1      1 920 ppm2     2 418
ASSI { 1432}
   (  segid "BrD " and resid 116  and name HG2%)
   (( segid "BrD " and resid 116  and name HA  ))
     2.500     1 600     1 600 peak  1432 weight  0 11000E+01 volume  0 32118E+03 ppm1      1 403 ppm2     4 823
ASSI { 1442}
   (  segid "BrD " and resid 116  and name HG2%)
   (( segid "BrD " and resid 116  and name HB  ))
     2 300     1 300     1.300 peak  1442 weight  0 11000E+01 volume  0 50062E+03 ppm1      1 403 ppm2     2 419
ASSI { 1452}
   (  segid "BrD " and resid 116  and name HD1%)
   (( segid "BrD " and resid 116  and name HG12))
     2 100     1 100     1 100 peak  1452 weight  0 11000E+01 volume  0 85569E+03 ppm1      1 399 ppm2     1 554
ASSI { 1462}
   (  segid "BrD " and resid 116  and name HD1%)
   (( segid "BrD " and resid 116  and name HG11))
     2.500     1 600     1 600 peak  1462 weight  0 11000E+01 volume  0 33669E+03 ppm1      1.399 ppm2     1 919
ASSI { 1512}
   (( segid "BrD " and resid 110  and name HB  ))
   (( segid "BrD " and resid 110  and name HA  ))
     2.400     1 400     1.400 peak  1512 weight  0.11000E+01 volume  0.40202E+03 ppm1      2 338 ppm2     4 418
ASSI { 1542}
   (  segid "BrD " and resid 110  and name HG2%)
   (( segid "BrD " and resid 110  and name HA  ))
     2.200     1 200     1 200 peak  1542 weight  0 11000E+01 volume  0 74299E+03 ppm1      1 251 ppm2     4 418
ASSI { 1552}
   (  segid "BrD " and resid 110  and name HG2%)
   (( segid "BrD " and resid 110  and name HB  ))
     2.200     1 200     1 200 peak  1552 weight  0 11000E+01 volume  0 70453E+03 ppm1      1 252 ppm2     2.361
ASSI { 1562}
   (  segid "BrD " and resid 110  and name HG2%)
   (( segid "BrD " and resid 110  and name HG11))
     2.600     1 700     1 700 peak  1562 weight  0.11000E+01 volume  0.27736E+03 ppm1      1 253 ppm2     1 718
ASSI { 1572}
   (  segid "BrD " and resid 110  and name HG2%)
   (  segid "BrD " and resid 110  and name HD1%)
     2 000     1.000     1.000 peak  1572 weight  0 11000E+01 volume  0 13448E+04 ppm1      1 254 ppm2     1 141
ASSI { 1602}
   (  segid "BrD " and resid 110  and name HD1%)
   (( segid "BrD " and resid 110  and name HA  ))
     2.200     1.200     1 200 peak  1602 weight  0 11000E+01 volume  0 74125E+03 ppm1      1.154 ppm2     4 420
ASSI { 1612}
   (  segid "BrD " and resid 110  and name HD1%)
   (( segid "BrD " and resid 110  and name HB  ))
     2 200     1 200     1 200 peak  1612 weight  0 11000E+01 volume  0 75209E+03 ppm1      1 154 ppm2     2 361
ASSI { 1622}
   (  segid "BrD " and resid 110  and name HD1%)
   (( segid "BrD " and resid 110  and name HG11))
     2.300     1 300     1 300 peak  1622 weight  0 11000E+01 volume  0 59823E+03 ppm1      1 154 ppm2     1.718
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DO2220" hTEOTS60

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ASSI { 1682}
  (  segid "BrD " and resid 50   and name HD1%)
  (( segid "BrD " and resid 50   and name HB  ))
     2.800     2.000     2 000 peak  1682 weight  0 11000E+01 volume  0 14989E+03 ppm1     1 154 ppm2     1 826
ASSI { 1692}
  (  segid "BrD " and resid 50   and name HD1%)
  (( segid "BrD " and resid 50   and name HG11))
     2 300     1 300     1 300 peak  1692 weight  0 11000E+01 volume  0 49711E+03 ppm1     1 154 ppm2     1 408
ASSI { 1702}
  (  segid "BrD " and resid 50   and name HD1%)
  (( segid "BrD " and resid 50   and name HG12))
     2 400     1 400     1 400 peak  1702 weight  0 11000E+01 volume  0 46662E+03 ppm1     1 155 ppm2     0.838
ASSI { 1712}
  (  segid "BrD " and resid 50   and name HD1%)
  (  segid "BrD " and resid 50   and name HG2%)
     2 400     1 400     1 400 peak  1712 weight  0 11000E+01 volume  0 45288E+03 ppm1     1 154 ppm2     0 994
ASSI { 1742}
  (  segid "BrD " and resid 50   and name HG2%)
  (( segid "BrD " and resid 50   and name HA  ))
     2.400     1 400     1 400 peak  1742 weight  0 11000E+01 volume  0 43004E+03 ppm1     1.006 ppm2     4 518
ASSI { 1752}
  (  segid "BrD " and resid 50   and name HG2%)
  (( segid "BrD " and resid 50   and name HB  ))
     2 200     1 200     1 200 peak  1752 weight  0 11000E+01 volume  0 61685E+03 ppm1     1 006 ppm2     1 825
ASSI { 1762}
  (  segid "BrD " and resid 50   and name HG2%)
  (( segid "BrD " and resid 50   and name HG11))
     2.800     2 000     2 000 peak  1762 weight  0 11000E+01 volume  0 16808E+03 ppm1     1.008 ppm2     1 409
ASSI { 1772}
  (  segid "BrD " and resid 50   and name HG2%)
  (( segid "BrD " and resid 50   and name HG12))
     2 400     1 400     1 400 peak  1772 weight  0 11000E+01 volume  0 40990E+03 ppm1     1 006 ppm2     0 838
ASSI { 1792}
  (( segid "BrD " and resid 101  and name HA  ))
  (  segid "BrD " and resid 101  and name HD1%)
     2 700     1 800     1 800 peak  1792 weight  0 11000E+01 volume  0 20691E+03 ppm1     4 261 ppm2     1 578
ASSI { 1812}
  (( segid "BrD " and resid 101  and name HB  ))
  (  segid "BrD " and resid 101  and name HD1%)
     2 300     1.300     1 300 peak  1812 weight  0 11000E+01 volume  0 50350E+03 ppm1     2 537 ppm2     1 578
ASSI { 1852}
  (( segid "BrD " and resid 101  and name HG11))
  (  segid "BrD " and resid 101  and name HG2%)
     2 600     1 700     1.700 peak  1852 weight  0 11000E+01 volume  0 23958E+03 ppm1     2 444 ppm2     1 609
ASSI { 1872}
  (  segid "BrD " and resid 101  and name HG2%)
  (( segid "BrD " and resid 101  and name HA  ))
     2 400     1 400     1 400 peak  1872 weight  0 11000E+01 volume  0 44349E+03 ppm1     1 596 ppm2     4 265
ASSI { 1882}
  (  segid "BrD " and resid 101  and name HG2%)
  (( segid "BrD " and resid 101  and name HB  ))
     2 200     1 200     1 200 peak  1882 weight  0.11000E+01 volume  0 72150E+03 ppm1     1.600 ppm2     2 536
ASSI { 1892}
  (  segid "BrD " and resid 101  and name HG2%)
  (( segid "BrD " and resid 101  and name HG12))
     2 300     1.300     1 300 peak  1892 weight  0 11000E+01 volume  0 60307E+03 ppm1     1 598 ppm2     1 806
ASSI { 1922}
  (  segid "BrD " and resid 101  and name HD1%)
  (( segid "BrD " and resid 101  and name HG11))
     2 300     1.300     1.300 peak  1922 weight  0 11000E+01 volume  0 50142E+03 ppm1     1 550 ppm2     2 467
ASSI { 1932}
  (  segid "BrD " and resid 101  and name HD1%)
  (( segid "BrD " and resid 101  and name HG12))
     2 200     1.200     1 200 peak  1932 weight  0 11000E+01 volume  0.71179E+03 ppm1     1 550 ppm2     1.806
ASSI { 1952}
  (( segid "BrD " and resid 21   and name HA  ))
  (  segid "BrD " and resid 21   and name HD1%)
     2 800     2 000     2.000 peak  1952 weight  0 11000E+01 volume  0 16491E+03 ppm1     4 359 ppm2     1 221
ASSI { 1962}
  (( segid "BrD " and resid 21   and name HB  ))
  (  segid "BrD " and resid 21   and name HG2%)
     3 100     2 400     2 400 peak  1962 weight  0 11000E+01 volume  0 84008E+02 ppm1     2 487 ppm2     1 588
ASSI { 1982}
  (( segid "BrD " and resid 21   and name HG12))
  (  segid "BrD " and resid 21   and name HD1%)
     2 500     1 600     1 600 peak  1982 weight  0 11000E+01 volume  0 32478E+03 ppm1     1 648 ppm2     1 222
ASSI { 2012}
  (  segid "BrD " and resid 21   and name HG2%)
  (( segid "BrD " and resid 21   and name HG11))
     2 600     1 700     1.700 peak  2012 weight  0.11000E+01 volume  0 24142E+03 ppm1     1.598 ppm2     2.357
ASSI { 2022}
  (  segid "BrD " and resid 21   and name HD1%)
  (( segid "BrD " and resid 21   and name HB  ))
     2.500     1 600     1.600 peak  2022 weight  0.11000E+01 volume  0 29587E+03 ppm1     1.206 ppm2     2 508
ASSI { 2032}
  (  segid "BrD " and resid 21   and name HD1%)
  (( segid "BrD " and resid 21   and name HG11))
     2.400     1 400     1 400 peak  2032 weight  0 11000E+01 volume  0 44094E+03 ppm1     1.205 ppm2     2 355
ASSI { 2042}
  (  segid "BrD " and resid 21   and name HD1%)
  (  segid "BrD " and resid 21   and name HG2%)
     2 300     1.300     1 300 peak  2042 weight  0 11000E+01 volume  0 49870E+03 ppm1     1 205 ppm2     1 588
ASSI { 2052}
  (( segid "BrD " and resid 112  and name HA  ))
  (( segid "BrD " and resid 112  and name HG1 ))
     2 700     1.800     1 800 peak  2052 weight  0 11000E+01 volume  0 21076E+03 ppm1     4 607 ppm2     2.942
ASSI { 2072}
  (( segid "BrD " and resid 112  and name HB1 ))
  (( segid "BrD " and resid 112  and name HG1 ))
     2 300     1 300     1 300 peak  2072 weight  0 11000E+01 volume  0 51152E+03 ppm1     2 684 ppm2     2.947
ASSI { 2092}
  (( segid "BrD " and resid 94   and name HA  ))
  (( segid "BrD " and resid 94   and name HG1 ))
     2 700     1 800     1.800 peak  2092 weight  0 11000E+01 volume  0 21281E+03 ppm1     4 830 ppm2     3.127
ASSI { 2112}
  (( segid "BrD " and resid 92   and name HG1 ))
  (( segid "BrD " and resid 92   and name HA  ))
     2 400     1 400     1 400 peak  2112 weight  0 11000E+01 volume  0.46860E+03 ppm1     2 816 ppm2     4 798
ASSI { 2142}
  (( segid "BrD " and resid 87   and name HG1 ))
  (( segid "BrD " and resid 87   and name HA  ))
     2 900     2 100     2 100 peak  2142 weight  0 11000E+01 volume  0.13435E+03 ppm1     3 030 ppm2     4.874
ASSI { 2152}
  (( segid "BrD " and resid 87   and name HG2 ))
  (( segid "BrD " and resid 87   and name HA  ))
     2 500     1 600     1 600 peak  2152 weight  0.11000E+01 volume  0 35437E+03 ppm1     2 782 ppm2     4 875
ASSI { 2172}
  (( segid "BrD " and resid 61   and name HG1 ))
  (( segid "BrD " and resid 61   and name HA  ))
     2 300     1 300     1 300 peak  2172 weight  0 11000E+01 volume  0 47499E+03 ppm1     2 980 ppm2     4 670
ASSI { 2182}
  (( segid "BrD " and resid 61   and name HG2 ))
  (( segid "BrD " and resid 61   and name HA  ))
     2 800     2 000     2 000 peak  2182 weight  0 11000E+01 volume  0 17452E+03 ppm1     2 832 ppm2     4 670
ASSI { 2202}
  (( segid "BrD " and resid 42   and name HG1 ))
  (( segid "BrD " and resid 42   and name HA  ))
     2 400     1 400     1.400 peak  2202 weight  0 11000E+01 volume  0 43794E+03 ppm1     2 880 ppm2     5 049
ASSI { 2222}
  (( segid "BrD " and resid 36   and name HG1 ))
  (( segid "BrD " and resid 36   and name HA  ))
     2 600     1 700     1 700 peak  2222 weight  0 11000E+01 volume  0 28226E+03 ppm1     2 781 ppm2     5 445
ASSI { 2252}
  (( segid "BrD " and resid 79   and name HG1 ))
  (( segid "BrD " and resid 79   and name HA  ))
     2 600     1 700     1 700 peak  2252 weight  0 11000E+01 volume  0 27675E+03 ppm1     3 033 ppm2     4 417
ASSI { 2262}
  (( segid "BrD " and resid 29   and name HA  ))
  (( segid "BrD " and resid 29   and name HB1 ))
     2 000     1 000     1 000 peak  2262 weight  0 11000E+01 volume  0 11521E+04 ppm1     4 810 ppm2     2 738
ASSI { 2272}
  (( segid "BrD " and resid 29   and name HG1 ))
  (( segid "BrD " and resid 29   and name HA  ))
     2 600     1 700     1 700 peak  2272 weight  0 11000E+01 volume  0.24467E+03 ppm1     2 980 ppm2     4 810
ASSI { 2302}
  (( segid "BrD " and resid 23   and name HG1 ))
  (( segid "BrD " and resid 23   and name HA  ))
     2 500     1 600     1 600 peak  2302 weight  0 11000E+01 volume  0 32948E+03 ppm1     3.124 ppm2     4 638
ASSI { 2312}
  (( segid "BrD " and resid 23   and name HG2 ))
  (( segid "BrD " and resid 23   and name HA  ))
     2 400     1 400     1 400 peak  2312 weight  0 11000E+01 volume  0.37520E+03 ppm1     3 068 ppm2     4 638
ASSI { 2322}
  (( segid "BrD " and resid 80   and name HD2 ))
  (( segid "BrD " and resid 80   and name HG1 ))
     2 500     1 600     1 600 peak  2322 weight  0 11000E+01 volume  0 34874E+03 ppm1     3 913 ppm2     2.347
ASSI { 2342}
  (( segid "BrD " and resid 80   and name HD2 ))
  (( segid "BrD " and resid 80   and name HB1 ))
     2.800     2 000     2.000 peak  2342 weight  0.11000E+01 volume  0 17327E+03 ppm1     3 913 ppm2     2 573
ASSI { 2372}
  (( segid "BrD " and resid 66   and name HA  ))
  (( segid "BrD " and resid 66   and name HD1 ))
     2 700     1 800     1 800 peak  2372 weight  0 11000E+01 volume  0 22458E+03 ppm1     5 000 ppm2     3 670
ASSI { 2382}
  (( segid "BrD " and resid 66   and name HG2 ))
  (( segid "BrD " and resid 66   and name HD1 ))
     2.500     1 600     1.600 peak  2382 weight  0 11000E+01 volume  0 35872E+03 ppm1     2 140 ppm2     3.670
ASSI { 2392}
  (( segid "BrD " and resid 9    and name HD1 ))
  (( segid "BrD " and resid 9    and name HG1 ))
     2 300     1 300     1 300 peak  2392 weight  0 11000E+01 volume  0.51278E+03 ppm1     3 769 ppm2     2 279
ASSI { 2432}
  (( segid "BrD " and resid 35   and name HG1 ))
  (( segid "BrD " and resid 35   and name HA  ))
     2 900     2 100     2 100 peak  2432 weight  0 11000E+01 volume  0 13495E+03 ppm1     3 422 ppm2     4.901
ASSI { 2442}
  (( segid "BrD " and resid 102  and name HB1 ))
  (( segid "BrD " and resid 102  and name HA  ))
     2 700     1 800     1.800 peak  2442 weight  0 11000E+01 volume  0 22859E+03 ppm1     1 994 ppm2     4 282
ASSI { 2452}
  (( segid "BrD " and resid 102  and name HB2 ))
  (( segid "BrD " and resid 102  and name HA  ))
     2.700     1 800     1 800 peak  2452 weight  0 11000E+01 volume  0.18482E+03 ppm1     1 848 ppm2     4 280
ASSI { 2462}
  (( segid "BrD " and resid 102  and name HB1 ))
  (  segid "BrD " and resid 102  and name HD1%)
     2 500     1 600     1 600 peak  2462 weight  0 11000E+01 volume  0 28966E+03 ppm1     1 992 ppm2     1 325
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ASSI { 2472}
  (( segid "BrD " and resid 102  and name HB2 ))
  (  segid "BrD " and resid 102  and name HD1%)
    2 500    1 600    1 600 peak  2472 weight  0 11000E+01 volume  0.33733E+03 ppm1    1 842 ppm2    1 325
ASSI { 2532}
  (( segid "BrD " and resid 73   and name HA  ))
  (( segid "BrD " and resid 73   and name HB2 ))
    2 500    1 600    1 600 peak  2532 weight  0 11000E+01 volume  0 31007E+03 ppm1    4 805 ppm2    2 482
ASSI { 2542}
  (( segid "BrD " and resid 73   and name HA  ))
  (( segid "BrD " and resid 73   and name HG  ))
    2 600    1 700    1 700 peak  2542 weight  0 11000E+01 volume  0 27034E+03 ppm1    4.805 ppm2    2 368
ASSI { 2572}
  (( segid "BrD " and resid 73   and name HB2 ))
  (  segid "BrD " and resid 73   and name HD1%)
    2 400    1 400    1 400 peak  2572 weight  0 11000E+01 volume  0 37597E+03 ppm1    2 487 ppm2    1 539
ASSI { 2582}
  (  segid "BrD " and resid 73   and name HD2%)
  (( segid "BrD " and resid 73   and name HA  ))
    2 200    1 200    1 200 peak  2582 weight  0 11000E+01 volume  0 64867E+03 ppm1    1 499 ppm2    4 827
ASSI { 2592}
  (  segid "BrD " and resid 73   and name HD2%)
  (( segid "BrD " and resid 73   and name HG  ))
    2 100    1 100    1 100 peak  2592 weight  0 11000E+01 volume  0 88262E+03 ppm1    1 500 ppm2    2 367
ASSI { 2602}
  (  segid "BrD " and resid 56   and name HD2%)
  (( segid "BrD " and resid 56   and name HG  ))
    2 200    1 200    1 200 peak  2602 weight  0 11000E+01 volume  0 64971E+03 ppm1    1 254 ppm2    2 328
ASSI { 2612}
  (  segid "BrD " and resid 56   and name HD2%)
  (( segid "BrD " and resid 56   and name HB1 ))
    2 700    1 800    1 800 peak  2612 weight  0 11000E+01 volume  0 20000E+03 ppm1    1 254 ppm2    2 703
ASSI { 2622}
  (  segid "BrD " and resid 56   and name HD2%)
  (( segid "BrD " and resid 56   and name HA  ))
    2 200    1 200    1 200 peak  2622 weight  0 11000E+01 volume  0 63602E+03 ppm1    1 253 ppm2    4 630
ASSI { 2652}
  (( segid "BrD " and resid 22   and name HB1 ))
  (( segid "BrD " and resid 22   and name HA  ))
    2 400    1 400    1 400 peak  2652 weight  0 11000E+01 volume  0 44257E+03 ppm1    2 682 ppm2    4 723
ASSI { 2662}
  (( segid "BrD " and resid 22   and name HB2 ))
  (( segid "BiD " and resid 22   and name HA  ))
    2 400    1 400    1 400 peak  2662 weight  0 11000E+01 volume  0 37194E+03 ppm1    2 287 ppm2    4 723
ASSI { 2682}
  (  segid "BrD " and resid 22   and name HD2%)
  (( segid "BrD " and resid 22   and name HA  ))
    2 200    1 200    1 200 peak  2682 weight  0 11000E+01 volume  0 64884E+03 ppm1    1 599 ppm2    4 723
ASSI { 2702}
  (( segid "BrD " and resid 63   and name HA  ))
  (( segid "BrD " and resid 63   and name HB1 ))
    2 900    2 100    2 100 peak  2702 weight  0 11000E+01 volume  0 13727E+03 ppm1    5 296 ppm2    2 907
ASSI { 2712}
  (( segid "BrD " and resid 63   and name HA  ))
  (( segid "BrD " and resid 63   and name HB2 ))
    2 700    1.800    1 800 peak  2712 weight  0 11000E+01 volume  0 18645E+03 ppm1    5 296 ppm2    2 535
ASSI { 2722}
  (( segid "BrD " and resid 63   and name HA  ))
  (( segid "BrD " and resid 63   and name HG  ))
    2 900    2 100    2 100 peak  2722 weight  0 11000E+01 volume  0.13509E+03 ppm1    5.293 ppm2    2.423
ASSI { 2732}
  (( segid "BrD " and resid 63   and name HA  ))
  (  segid "BrD " and resid 63   and name HD1%)
    2 700    1 800    1 800 peak  2732 weight  0 11000E+01 volume  0 22485E+03 ppm1    5 296 ppm2    1 649
ASSI { 2742}
  (( segid "BrD " and resid 63   and name HA  ))
  (  segid "BrD " and resid 63   and name HD2%)
    3 300    2 700    2 200 peak  2742 weight  0 11000E+01 volume  0 65439E+02 ppm1    5 296 ppm2    1 490
ASSI { 2752}
  (( segid "BrD " and resid 63   and name HB2 ))
  (  segid "BrD " and resid 63   and name HD1%)
    2 500    1 600    1 600 peak  2752 weight  0.11000E+01 volume  0 34992E+03 ppm1    2 538 ppm2    1.653
ASSI { 2762}
  (( segid "BrD " and resid 63   and name HB2 ))
  (  segid "BrD " and resid 63   and name HD2%)
    2 700    1 800    1 800 peak  2762 weight  0 11000E+01 volume  0 19887E+03 ppm1    2 538 ppm2    1 491
ASSI { 2772}
  (( segid "BrD " and resid 63   and name HB1 ))
  (  segid "BrD " and resid 63   and name HD1%)
    2 600    1 700    1 700 peak  2772 weight  0 11000E+01 volume  0 26127E+03 ppm1    2 883 ppm2    1 653
ASSI { 2782}
  (( segid "BrD " and resid 63   and name HB1 ))
  (  segid "BrD " and resid 63   and name HD2%)
    2 600    1 700    1 700 peak  2782 weight  0 11000E+01 volume  0 25187E+03 ppm1    2 883 ppm2    1 491
ASSI { 2852}
  (  segid "BrD " and resid 14   and name HD2%)
  (( segid "BrD " and resid 14   and name HA  ))
    3 100    2 400    2 400 peak  2852 weight  0 11000E+01 volume  0 89872E+02 ppm1    1.400 ppm2    4 655
ASSI { 2862}
  (  segid "BrD " and resid 14   and name HD2%)
  (( segid "BrD " and resid 14   and name HG  ))
    2.700    1 800    1.800 peak  2862 weight  0 11000E+01 volume  0 20094E+03 ppm1    1 401 ppm2    2.061
ASSI { 2872}
  (( segid "BrD " and resid 24   and name HA  ))
  (( segid "BrD " and resid 24   and name HG1 ))
    2 700    1 800    1.800 peak  2872 weight  0.11000E+01 volume  0 22636E+03 ppm1    4 783 ppm2    3 454
ASSI { 2892}
  (( segid "BrD " and resid 24   and name HG2 ))
  (( segid "BrD " and resid 24   and name HA  ))
    2 400    1 400    1 400 peak  2892 weight  0 11000E+01 volume  0 36992E+03 ppm1    3.076 ppm2    4 784
ASSI { 2902}
  (( segid "BrD " and resid 83   and name HB  ))
  (( segid "BrD " and resid 83   and name HA  ))
    2.300    1 300    1 300 peak  2902 weight  0 11000E+01 volume  0 54241E+03 ppm1    4 804 ppm2    4.460
ASSI { 2912}
  (( segid "BrD " and resid 17   and name HA  ))
  (( segid "BrD " and resid 17   and name HB  ))
    2 500    1 600    1.600 peak  2912 weight  0 11000E+01 volume  0 32083E+03 ppm1    4 542 ppm2    4 860
ASSI { 2932}
  (  segid "BrD " and resid 25   and name HG2%)
  (( segid "BrD " and resid 25   and name HB  ))
    2 300    1 300    1 300 peak  2932 weight  0 11000E+01 volume  0 60381E+03 ppm1    1.650 ppm2    3 005
ASSI { 2942}
  (  segid "BrD " and resid 25   and name HG1%)
  (( segid "BrD " and resid 25   and name HB  ))
    2.200    1 200    1 200 peak  2942 weight  0 11000E+01 volume  0.72430E+03 ppm1    1 795 ppm2    3 006
ASSI { 2972}
  (( segid "BrD " and resid 49   and name HA  ))
  (( segid "BrD " and resid 49   and name HB  ))
    2 500    1 600    1 600 peak  2972 weight  0 11000E+01 volume  0 32061E+03 ppm1    4 658 ppm2    2 620
ASSI { 2992}
  (( segid "BrD " and resid 49   and name HA  ))
  (  segid "BrD " and resid 49   and name HG2%)
    2 900    2 100    2 100 peak  2992 weight  0 11000E+01 volume  0 13480E+03 ppm1    4 658 ppm2    1 570
ASSI { 3012}
  (( segid "BrD " and resid 49   and name HB  ))
  (  segid "BrD " and resid 49   and name HG2%)
    2 500    1 600    1 600 peak  3012 weight  0 11000E+01 volume  0 36520E+03 ppm1    2 634 ppm2    1 570
ASSI { 3022}
  (  segid "BrD " and resid 49   and name HG1%)
  (( segid "BrD " and resid 49   and name HB  ))
    2 500    1 600    1 600 peak  3022 weight  0 11000E+01 volume  0 34642E+03 ppm1    1 647 ppm2    2 615
ASSI { 3042}
  (  segid "BrD " and resid 49   and name HG1%)
  (( segid "BrD " and resid 49   and name HA  ))
    2 700    1.800    1 800 peak  3042 weight  0 11000E+01 volume  0.21850E+03 ppm1    1 647 ppm2    4 679
ASSI { 3052}
  (  segid "BrD " and resid 69   and name HG1%)
  (( segid "BrD " and resid 69   and name HA  ))
    2 100    1 100    1 100 peak  3052 weight  0 11000E+01 volume  0 91954E+03 ppm1    1 550 ppm2    4.695
ASSI { 3072}
  (( segid "BrD " and resid 58   and name HA  ))
  (( segid "BrD " and resid 58   and name HB  ))
    2 200    1 200    1 200 peak  3072 weight  0 11000E+01 volume  0.67241E+03 ppm1    4 456 ppm2    4 703
ASSI { 3102}
  (( segid "BrD " and resid 28   and name HB2 ))
  (( segid "BrD " and resid 28   and name HA  ))
    2 800    2 000    2 000 peak  3102 weight  0 11000E+01 volume  0 15370E+03 ppm1    3 372 ppm2    4 582
ASSI { 3112}
  (( segid "BrD " and resid 28   and name HB1 ))
  (( segid "BrD " and resid 28   and name HA  ))
    2 800    2 000    2 000 peak  3112 weight  0 11000E+01 volume  0.16666E+03 ppm1    3 571 ppm2    4 582
ASSI { 3142}
  (( segid "BrD " and resid 64   and name HA  ))
  (( segid "BrD " and resid 64   and name HD1 ))
    3 000    2 200    2 200 peak  3142 weight  0 11000E+01 volume  0 11363E+03 ppm1    4.950 ppm2    2 373
ASSI { 3162}
  (( segid "BrD " and resid 64   and name HB1 ))
  (( segid "BrD " and resid 64   and name HA  ))
    2.200    1 200    1 200 peak  3162 weight  0 11000E+01 volume  0 77951E+03 ppm1    2.636 ppm2    4 940
ASSI { 3172}
  (( segid "BrD " and resid 64   and name HG1 ))
  (( segid "BrD " and resid 64   and name HA  ))
    2 500    1 600    1 600 peak  3172 weight  0 11000E+01 volume  0 29624E+03 ppm1    2 190 ppm2    4 938
ASSI { 3182}
  (( segid "BrD " and resid 64   and name HG1 ))
  (( segid "BrD " and resid 64   and name HB1 ))
    2.300    1 300    1.300 peak  3182 weight  0 11000E+01 volume  0.60420E+03 ppm1    2 190 ppm2    2 662
ASSI { 3192}
  (( segid "BrD " and resid 64   and name HG1 ))
  (( segid "BrD " and resid 64   and name HE1 ))
    2.500    1 600    1 600 peak  3192 weight  0 11000E+01 volume  0 31904E+03 ppm1    2 190 ppm2    3 597
ASSI { 3202}
  (( segid "BrD " and resid 6    and name HB1 ))
  (( segid "BrD " and resid 6    and name HA  ))
    2 400    1 400    1 400 peak  3202 weight  0.11000E+01 volume  0 45358E+03 ppm1    2 489 ppm2    4 969
ASSI { 3212}
  (( segid "BrD " and resid 6    and name HD1 ))
  (( segid "BrD " and resid 6    and name HA  ))
    2 800    2 000    2 000 peak  3212 weight  0 11000E+01 volume  0 15911E+03 ppm1    2 310 ppm2    4 972
ASSI { 3222}
  (( segid "BrD " and resid 6    and name HG2 ))
  (( segid "BrD " and resid 6    and name HA  ))
    2 900    2 100    2 100 peak  3222 weight  0 11000E+01 volume  0 13404E+03 ppm1    2 040 ppm2    4 973
ASSI { 3232}
  (( segid "BrD " and resid 104  and name HG1 ))
  (( segid "BrD " and resid 104  and name HA  ))
    2.400    1 400    1 400 peak  3232 weight  0 11000E+01 volume  0 41964E+03 ppm1    2 140 ppm2    4 672
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ASSI { 3242}
  (( segid "BrD " and resid 104  and name HA  ))
  (( segid "BrD " and resid 104  and name HB1 ))
     2.100    1 100     1 100 peak  3242 weight  0 11000E+01 volume  0 87442E+03 ppm1    4 657 ppm2    2 537
ASSI { 3272}
  (( segid "BrD " and resid 104  and name HA  ))
  (( segid "BrD " and resid 107  and name HB1 ))
     2.500    1 600     1 600 peak  3272 weight  0 11000E+01 volume  0.31692E+03 ppm1    4 656 ppm2    3 663
ASSI { 3292}
  (( segid "BrD " and resid 111  and name HB2 ))
  (( segid "BrD " and resid 111  and name HA  ))
     2 100    1 100     1 100 peak  3292 weight  0 11000E+01 volume  0.10458E+04 ppm1    2 366 ppm2    4 656
ASSI { 3312}
  (( segid "BrD " and resid 111  and name HA  ))
  (( segid "BrD " and resid 111  and name HG2 ))
     2 800    2 000     2 000 peak  3312 weight  0 11000E+01 volume  0 17232E+03 ppm1    4 656 ppm2    1 918
ASSI { 3332}
  (( segid "BrD " and resid 111  and name HA  ))
  (( segid "BrD " and resid 111  and name HB1 ))
     2 100    1 100     1 100 peak  3332 weight  0 11000E+01 volume  0 97545E+03 ppm1    4 656 ppm2    2.473
ASSI { 3362}
  (( segid "BrD " and resid 19   and name HA  ))
  (( segid "BrD " and resid 19   and name HD1 ))
     3 100    2 400     2 400 peak  3362 weight  0 11000E+01 volume  0 91418E+02 ppm1    4 310 ppm2    2 214
ASSI { 3372}
  (( segid "BrD " and resid 19   and name HB1 ))
  (( segid "BrD " and resid 19   and name HA  ))
     2 500    1 600     1 600 peak  3372 weight  0 11000E+01 volume  0 34161E+03 ppm1    2 290 ppm2    4 297
ASSI { 3382}
  (( segid "BrD " and resid 19   and name HB1 ))
  (( segid "BrD " and resid 16   and name HA  ))
     3 900    3 800     1.600 peak  3382 weight  0 11000E+01 volume  0 22305E+02 ppm1    2.290 ppm2    4 507
ASSI { 3392}
  (( segid "BrD " and resid 19   and name HG1 ))
  (( segid "BrD " and resid 19   and name HA  ))
     2 400    1 400     1 400 peak  3392 weight  0 11000E+01 volume  0 37229E+03 ppm1    1.895 ppm2    4 296
ASSI { 3402}
  (( segid "BrD " and resid 19   and name HG1 ))
  (( segid "BrD " and resid 19   and name HE1 ))
     2 600    1 700     1 700 peak  3402 weight  0 11000E+01 volume  0 28547E+03 ppm1    1 895 ppm2    3 526
ASSI { 3412}
  (( segid "BrD " and resid 19   and name HD1 ))
  (( segid "BrD " and resid 19   and name HE1 ))
     1 800    0 800     0 800 peak  3412 weight  0 11000E+01 volume  0 21730E+04 ppm1    2 192 ppm2    3 522
ASSI { 3422}
  (( segid "BrD " and resid 60   and name HA  ))
  (( segid "BrD " and resid 60   and name HB1 ))
     1 700    0 700     0 700 peak  3422 weight  0 11000E+01 volume  0 29577E+04 ppm1    4 805 ppm2    4 995
ASSI { 3452}
  (( segid "BrD " and resid 11   and name HB1 ))
  (( segid "BrD " and resid 11   and name HA  ))
     2 300    1 300     1 300 peak  3452 weight  0 11000E+01 volume  0 52164E+03 ppm1    2 933 ppm2    4 942
ASSI { 3462}
  (( segid "BrD " and resid 11   and name HB2 ))
  (( segid "BrD " and resid 11   and name HA  ))
     2 300    1 300     1.300 peak  3462 weight  0 11000E+01 volume  0 61125E+03 ppm1    2 586 ppm2    4.943
ASSI { 3492}
  (( segid "BrD " and resid 97   and name HA  ))
  (( segid "BrD " and resid 97   and name HB1 ))
     2 300    1 300     1.300 peak  3492 weight  0 11000E+01 volume  0 52974E+03 ppm1    4 805 ppm2    2 704
ASSI { 3532}
  (( segid "BrD " and resid 109  and name HE2 ))
  (( segid "BrD " and resid 109  and name HD1 ))
     2 500    1 600     1 600 peak  3532 weight  0 11000E+01 volume  0.30326E+03 ppm1    3 029 ppm2    1 994
ASSI { 3542}
  (( segid "BrD " and resid 109  and name HE2 ))
  (( segid "BrD " and resid 109  and name HG1 ))
     2 700    1 800     1.800 peak  3542 weight  0 11000E+01 volume  0 22719E+03 ppm1    3 027 ppm2    1 411
ASSI { 3552}
  (( segid "BrD " and resid 109  and name HE1 ))
  (( segid "BrD " and resid 109  and name HG1 ))
     2 600    1 700     1 700 peak  3552 weight  0 11000E+01 volume  0 23490E+03 ppm1    3 176 ppm2    1.411
ASSI { 3562}
  (( segid "BrD " and resid 109  and name HD1 ))
  (( segid "BrD " and resid 109  and name HE1 ))
     2 700    1 800     1 800 peak  3562 weight  0 11000E+01 volume  0 22693E+03 ppm1    1 994 ppm2    3.195
ASSI { 3602}
  (( segid "BrD " and resid 86   and name HE1 ))
  (( segid "BrD " and resid 86   and name HG2 ))
     2 900    2 100     2 100 peak  3602 weight  0 11000E+01 volume  0 13036E+03 ppm1    3 080 ppm2    0 766
ASSI { 3612}
  (( segid "BrD " and resid 86   and name HD1 ))
  (( segid "BrD " and resid 86   and name HG2 ))
     2 300    1 300     1.300 peak  3612 weight  0 11000E+01 volume  0 49629E+03 ppm1    1 896 ppm2    0 765
ASSI { 3622}
  (( segid "BrD " and resid 86   and name HD1 ))
  (( segid "BrD " and resid 86   and name HE1 ))
     2 600    1 700     1 700 peak  3622 weight  0.11000E+01 volume  0 24556E+03 ppm1    1 892 ppm2    3 093
ASSI { 3632}
  (( segid "BrD " and resid 86   and name HA  ))
  (( segid "BrD " and resid 86   and name HG1 ))
     2 800    2 000     2 000 peak  3632 weight  0 11000E+01 volume  0 14893E+03 ppm1    4 806 ppm2    1 895
ASSI { 3682}
  (( segid "BrD " and resid 8    and name HG1 ))
  (( segid "BrD " and resid 8    and name HD1 ))
     2 000    1 000     1.000 peak  3682 weight  0 11000E+01 volume  0.11498E+04 ppm1    2 635 ppm2    4 436
ASSI { 3692}
  (( segid "BrD " and resid 8    and name HG1 ))
  (( segid "BrD " and resid 8    and name HD2 ))
     2.100    1 100     1 100 peak  3692 weight  0.11000E+01 volume  0 87712E+03 ppm1    2 635 ppm2    4 286
ASSI { 3702}
  (( segid "BrD " and resid 8    and name HB2 ))
  (( segid "BrD " and resid 8    and name HA  ))
     2 600    1 700     1 700 peak  3702 weight  0 11000E+01 volume  0 24482E+03 ppm1    2.487 ppm2    5 021
ASSI { 3712}
  (( segid "BrD " and resid 8    and name HB1 ))
  (( segid "BrD " and resid 8    and name HA  ))
     2.400    1 400     1.400 peak  3712 weight  0 11000E+01 volume  0 36862E+03 ppm1    2 831 ppm2    5 021
ASSI { 3722}
  (( segid "BrD " and resid 8    and name HD1 ))
  (( segid "BrD " and resid 7    and name HA  ))
     2 100    1 100     1 100 peak  3722 weight  0 11000E+01 volume  0 89203E+03 ppm1    4 407 ppm2    5 144
ASSI { 3732}
  (( segid "BrD " and resid 8    and name HD2 ))
  (( segid "BrD " and resid 7    and name HA  ))
     2 100    1 100     1 100 peak  3732 weight  0 11000E+01 volume  0.93259E+03 ppm1    4 263 ppm2    5.144
ASSI { 3752}
  (( segid "BrD " and resid 44   and name HA  ))
  (( segid "BrD " and resid 44   and name HB1 ))
     2 400    1 400     1.400 peak  3752 weight  0 11000E+01 volume  0 42716E+03 ppm1    5 098 ppm2    2 973
ASSI { 3762}
  (( segid "BrD " and resid 44   and name HA  ))
  (( segid "BrD " and resid 44   and name HB2 ))
     2 600    1 700     1.700 peak  3762 weight  0 11000E+01 volume  0 27521E+03 ppm1    5 098 ppm2    2 636
ASSI { 3792}
  (( segid "BrD " and resid 44   and name HB2 ))
  (( segid "BrD " and resid 44   and name HD1 ))
     2 800    2 000     2 000 peak  3792 weight  0 11000E+01 volume  0 16780E+03 ppm1    2 631 ppm2    4 337
ASSI { 3802}
  (( segid "BrD " and resid 44   and name HB1 ))
  (( segid "BrD " and resid 44   and name HD1 ))
     3 200    2 600     2 300 peak  3802 weight  0.11000E+01 volume  0 70033E+02 ppm1    2 981 ppm2    4 337
ASSI { 3822}
  (( segid "BrD " and resid 44   and name HG1 ))
  (( segid "BrD " and resid 44   and name HA  ))
     2 900    2 100     2 100 peak  3822 weight  0 11000E+01 volume  0 14259E+03 ppm1    2 729 ppm2    5 114
ASSI { 3832}
  (( segid "BrD " and resid 44   and name HG2 ))
  (( segid "BrD " and resid 44   and name HA  ))
     2 700    1 800     1 800 peak  3832 weight  0 11000E+01 volume  0 22601E+03 ppm1    2 645 ppm2    5 114
ASSI { 3842}
  (( segid "BrD " and resid 41   and name HA  ))
  (( segid "BrD " and resid 41   and name HB  ))
     1 900    0 900     0.900 peak  3842 weight  0 11000E+01 volume  0 19310E+04 ppm1    4 657 ppm2    4 899
ASSI { 3882}
  (( segid "BrD " and resid 103  and name HG2 ))
  (( segid "BrD " and resid 103  and name HA  ))
     2 800    2 000     2 000 peak  3882 weight  0 11000E+01 volume  0 14970E+03 ppm1    2 519 ppm2    3 789
ASSI { 3892}
  (( segid "BrD " and resid 103  and name HG1 ))
  (( segid "BrD " and resid 103  and name HA  ))
     2 900    2.100     2 100 peak  3892 weight  0.11000E+01 volume  0 14619E+03 ppm1    2.598 ppm2    3 789
ASSI { 3912}
  (( segid "BrD " and resid 103  and name HG2 ))
  (( segid "BrD " and resid 103  and name HB1 ))
     3.000    2.200     2 200 peak  3912 weight  0 11000E+01 volume  0 10641E+03 ppm1    2 519 ppm2    2 346
ASSI { 3922}
  (( segid "BrD " and resid 103  and name HG1 ))
  (( segid "BrD " and resid 103  and name HB1 ))
     3 200    2.600     2 300 peak  3922 weight  0 11000E+01 volume  0 80668E+02 ppm1    2 598 ppm2    2 346
ASSI { 3942}
  (( segid "BrD " and resid 48   and name HA  ))
  (( segid "BrD " and resid 48   and name HG1 ))
     3.100    2 400     2 400 peak  3942 weight  0 11000E+01 volume  0.93117E+02 ppm1    4.803 ppm2    2 940
ASSI { 3952}
  (( segid "BrD " and resid 48   and name HA  ))
  (( segid "BrD " and resid 48   and name HG2 ))
     3 000    2 200     2.200 peak  3952 weight  0.11000E+01 volume  0.10971E+03 ppm1    4 803 ppm2    2.851
ASSI { 3982}
  (  segid "BrD " and resid 50   and name HD1%)
  (( segid "BrD " and resid 50   and name HA  ))
     2 300    1 300     1 300 peak  3982 weight  0 11000E+01 volume  0 51678E+03 ppm1    1 155 ppm2    4 518
ASSI { 4012}
  (  segid "BrD " and resid 110  and name HD1%)
  (( segid "BrD " and resid 110  and name HG12))
     2.600    1 700     1 700 peak  4012 weight  0.11000E+01 volume  0 27804E+03 ppm1    1 154 ppm2    1 652
ASSI { 4022}
  (  segid "BrD " and resid 110  and name HG2%)
  (( segid "BrD " and resid 110  and name HG12))
     2 500    1.600     1 600 peak  4022 weight  0 11000E+01 volume  0 35399E+03 ppm1    1.253 ppm2    1 651
ASSI { 4032}
  (( segid "BrD " and resid 110  and name HB  ))
  (( segid "BrD " and resid 110  and name HG12))
     3 300    2 700     2.200 peak  4032 weight  0 11000E+01 volume  0 60399E+02 ppm1    2 338 ppm2    1.651
ASSI { 4052}
  (( segid "BrD " and resid 24   and name HB1 ))
  (( segid "BrD " and resid 24   and name HG1 ))
     2.600    1 700     1 700 peak  4052 weight  0.11000E+01 volume  0 27715E+03 ppm1    3 076 ppm2    3.453
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ASSI { 4062}
  (( segid "BrD " and resid 80   and name HD1 ))
  (( segid "BrD " and resid 80   and name HG1 ))
   2.400    1 400    1.400 peak  4062 weight  0 11000E+01 volume  0 37330E+03 ppm1    3 956 ppm2    2 347
ASSI { 4072}
  (( segid "BrD " and resid 80   and name HD1 ))
  (( segid "BrD " and resid 80   and name HB1 ))
   2 700    1 800    1.800 peak  4072 weight  0 11000E+01 volume  0 22342E+03 ppm1    3 956 ppm2    2 573
ASSI { 4112}
  (( segid "BrD " and resid 101  and name HA  ))
  (( segid "BrD " and resid 101  and name HB  ))
   2 600    1 700    1 700 peak  4112 weight  0 11000E+01 volume  0 25152E+03 ppm1    4 263 ppm2    2 535
ASSI { 4122}
  (( segid "BrD " and resid 101  and name HA  ))
  (( segid "BrD " and resid 101  and name HG11))
   2 600    1 700    1 700 peak  4122 weight  0 11000E+01 volume  0 23036E+03 ppm1    4 263 ppm2    2 469
ASSI { 4132}
  (( segid "BrD " and resid 101  and name HA  ))
  (( segid "BrD " and resid 101  and name HG12))
   2 500    1.600    1.600 peak  4132 weight  0.11000E+01 volume  0 31941E+03 ppm1    4 261 ppm2    1 806
ASSI { 4142}
  (  segid "BrD " and resid 38   and name HG1%)
  (( segid "BrD " and resid 38   and name HA  ))
   2 300    1 300    1 300 peak  4142 weight  0 11000E+01 volume  0 50428E+03 ppm1    1.058 ppm2    4 168
ASSI { 4162}
  (  segid "BrD " and resid 81   and name HG2%)
  (( segid "BrD " and resid 81   and name HA  ))
   2 400    1 400    1 400 peak  4162 weight  0 11000E+01 volume  0 38926E+03 ppm1    0 761 ppm2    3.716
ASSI { 4182}
  (  segid "BrD " and resid 81   and name HG1%)
  (( segid "BrD " and resid 81   and name HA  ))
   2 400    1 400    1.400 peak  4182 weight  0 11000E+01 volume  0 43496E+03 ppm1    1 059 ppm2    3 716
ASSI { 4212}
  (( segid "BrD " and resid 69   and name HB  ))
  (( segid "BrD " and resid 69   and name HA  ))
   2 200    1 200    1.200 peak  4212 weight  0 11000E+01 volume  0 67869E+03 ppm1    2 929 ppm2    4 696
ASSI { 4222}
  (( segid "BrD " and resid 18   and name HA  ))
  (( segid "BrD " and resid 18   and name HB1 ))
   2 800    2 000    2 000 peak  4222 weight  0 11000E+01 volume  0 15123E+03 ppm1    3 866 ppm2    2 131
ASSI { 4272}
  (( segid "BrD " and resid 116  and name HB  ))
  (  segid "BrD " and resid 116  and name HD1%)
   2 500    1 600    1 600 peak  4272 weight  0 11000E+01 volume  0 31982E+03 ppm1    2 409 ppm2    1 399
ASSI { 4282}
  (( segid "BrD " and resid 110  and name HB  ))
  (( segid "BrD " and resid 110  and name HG11))
   3.100    2.400    2 400 peak  4282 weight  0 11000E+01 volume  0 90397E+02 ppm1    2 338 ppm2    1 718
ASSI { 4302}
  (( segid "BrD " and resid 50   and name HA  ))
  (( segid "BrD " and resid 50   and name HG11))
   2 600    1 700    1 700 peak  4302 weight  0 11000E+01 volume  0 24102E+03 ppm1    4 506 ppm2    1 409
ASSI { 4322}
  (( segid "BrD " and resid 50   and name HB  ))
  (( segid "BrD " and resid 50   and name HG12))
   2 700    1 800    1 800 peak  4322 weight  0 11000E+01 volume  0 20938E+03 ppm1    1 797 ppm2    0.840
ASSI { 4332}
  (( segid "BrD " and resid 50   and name HB  ))
  (( segid "BrD " and resid 50   and name HG11))
   2 700    1.800    1 800 peak  4332 weight  0 11000E+01 volume  0 20876E+03 ppm1    1 797 ppm2    1 407
ASSI { 4342}
  (( segid "BrD " and resid 50   and name HB  ))
  (( segid "BrD " and resid 50   and name HA  ))
   3.000    2 200    2 200 peak  4342 weight  0 11000E+01 volume  0 11875E+03 ppm1    1 797 ppm2    4 516
ASSI { 4382}
  (( segid "BrD " and resid 21   and name HA  ))
  (( segid "BrD " and resid 21   and name HB  ))
   2.700    1 800    1 800 peak  4382 weight  0 11000E+01 volume  0.19816E+03 ppm1    4 359 ppm2    2 515
ASSI { 4392}
  (( segid "BrD " and resid 21   and name HA  ))
  (( segid "BrD " and resid 21   and name HG12))
   2.600    1 700    1.700 peak  4392 weight  0 11000E+01 volume  0 25295E+03 ppm1    4 358 ppm2    1 653
ASSI { 4402}
  (( segid "BrD " and resid 21   and name HA  ))
  (( segid "BrD " and resid 21   and name HG11))
   2 600    1 700    1 700 peak  4402 weight  0 11000E+01 volume  0 24995E+03 ppm1    4 358 ppm2    2 357
ASSI { 4412}
  (( segid "BrD " and resid 21   and name HB  ))
  (( segid "BrD " and resid 21   and name HG11))
   2 900    2 100    2 100 peak  4412 weight  0 11000E+01 volume  0.13199E+03 ppm1    2 487 ppm2    2 356
ASSI { 4472}
  (( segid "BrD " and resid 21   and name HG12))
  (( segid "BrD " and resid 21   and name HB  ))
   2.800    2 000    2 000 peak  4472 weight  0 11000E+01 volume  0 17027E+03 ppm1    1 642 ppm2    2.511
ASSI { 4482}
  (( segid "BrD " and resid 21   and name HG12))
  (( segid "BrD " and resid 21   and name HG11))
   2 200    1 200    1.200 peak  4482 weight  0 11000E+01 volume  0.65087E+03 ppm1    1.642 ppm2    2.357
ASSI { 4502}
  (  segid "BrD " and resid 21   and name HG2%)
  (( segid "BrD " and resid 21   and name HA  ))
   2 400    1.400    1 400 peak  4502 weight  0 11000E+01 volume  0.39582E+03 ppm1    1 596 ppm2    4 369
ASSI { 4512}
  (( segid "BrD " and resid 36   and name HG1 ))
  (( segid "BrD " and resid 36   and name HB2 ))
   2.100    1.100    1.100 peak  4512 weight  0.11000E+01 volume  0 10618E+04 ppm1    2 781 ppm2    2 342
ASSI { 4562}
  (( segid "BrD " and resid 9    and name HG1 ))
  (( segid "BrD " and resid 9    and name HA  ))
   2 800    2 000    2.000 peak  4562 weight  0 11000E+01 volume  0 15274E+03 ppm1    2 236 ppm2    4 940
ASSI { 4582}
  (( segid "BrD " and resid 9    and name HA  ))
  (( segid "BrD " and resid 9    and name HB2 ))
   2 400    1 400    1 400 peak  4582 weight  0 11000E+01 volume  0 39636E+03 ppm1    4 953 ppm2    2 385
ASSI { 4592}
  (( segid "BrD " and resid 35   and name HB2 ))
  (( segid "BrD " and resid 35   and name HG1 ))
   2 600    1 700    1.700 peak  4592 weight  0 11000E+01 volume  0 27554E+03 ppm1    2 781 ppm2    3 447
ASSI { 4602}
  (( segid "BrD " and resid 35   and name HB1 ))
  (( segid "BrD " and resid 35   and name HG1 ))
   3 000    2 200    2 200 peak  4602 weight  0 11000E+01 volume  0 10522E+03 ppm1    2 838 ppm2    3 447
ASSI { 4632}
  (  segid "BrD " and resid 73   and name HD1%)
  (( segid "BrD " and resid 73   and name HG  ))
   2 100    1 100    1 100 peak  4632 weight  0.11000E+01 volume  0 81939E+03 ppm1    1 549 ppm2    2 368
ASSI { 4642}
  (( segid "BrD " and resid 56   and name HA  ))
  (( segid "BrD " and resid 56   and name HB1 ))
   2 500    1 600    1 600 peak  4642 weight  0 11000E+01 volume  0 31507E+03 ppm1    4 606 ppm2    2.694
ASSI { 4652}
  (  segid "BrD " and resid 22   and name HD2%)
  (( segid "BrD " and resid 22   and name HB1 ))
   2 500    1 600    1 600 peak  4652 weight  0 11000E+01 volume  0 35307E+03 ppm1    1 600 ppm2    2 702
ASSI { 4662}
  (( segid "BrD " and resid 22   and name HA  ))
  (( segid "BrD " and resid 22   and name HG  ))
   2 400    1 400    1 400 peak  4662 weight  0 11000E+01 volume  0 43065E+03 ppm1    4 704 ppm2    2 360
ASSI { 4722}
  (( segid "BrD " and resid 14   and name HA  ))
  (( segid "BrD " and resid 14   and name HB1 ))
   2 400    1 400    1 400 peak  4722 weight  0 11000E+01 volume  0 40350E+03 ppm1    4 655 ppm2    2 464
ASSI { 4732}
  (( segid "BrD " and resid 14   and name HA  ))
  (( segid "BrD " and resid 14   and name HB2 ))
   2 500    1 600    1.600 peak  4732 weight  0 11000E+01 volume  0 34201E+03 ppm1    4 655 ppm2    2 159
ASSI { 4742}
  (( segid "BrD " and resid 14   and name HA  ))
  (( segid "BrD " and resid 14   and name HG  ))
   2 800    2 000    2 000 peak  4742 weight  0 11000E+01 volume  0 16298E+03 ppm1    4 655 ppm2    2 062
ASSI { 4752}
  (  segid "BrD " and resid 14   and name HD2%)
  (( segid "BrD " and resid 14   and name HB2 ))
   2 900    2 100    2 100 peak  4752 weight  0 11000E+01 volume  0 12176E+03 ppm1    1 401 ppm2    2 155
ASSI { 4762}
  (  segid "BrD " and resid 14   and name HD2%)
  (( segid "BrD " and resid 14   and name HB1 ))
   2.200    1.200    1.200 peak  4762 weight  0 11000E+01 volume  0 78049E+03 ppm1    1 401 ppm2    2 466
ASSI { 4782}
  (( segid "BrD " and resid 24   and name HB2 ))
  (( segid "BrD " and resid 24   and name HG1 ))
   2 700    1 800    1 800 peak  4782 weight  0 11000E+01 volume  0.20235E+03 ppm1    2 989 ppm2    3 453
ASSI { 4812}
  (( segid "BrD " and resid 25   and name HA  ))
  (  segid "BrD " and resid 25   and name HG2%)
   2 600    1 700    1 700 peak  4812 weight  0 11000E+01 volume  0 28433E+03 ppm1    4 412 ppm2    1 637
ASSI { 4822}
  (  segid "BrD " and resid 25   and name HG1%)
  (( segid "BrD " and resid 25   and name HA  ))
   2 300    1 300    1 300 peak  4822 weight  0 11000E+01 volume  0 50491E+03 ppm1    1 796 ppm2    4 427
ASSI { 4832}
  (( segid "BrD " and resid 30   and name HB1 ))
  (( segid "BrD " and resid 30   and name HA  ))
   2.700    1 800    1 800 peak  4832 weight  0 11000E+01 volume  0 18839E+03 ppm1    4.907 ppm2    5 445
ASSI { 4852}
  (( segid "BrD " and resid 30   and name HA  ))
  (( segid "BrD " and resid 30   and name HB2 ))
   2 900    2 100    2 100 peak  4852 weight  0 11000E+01 volume  0 13412E+03 ppm1    5 444 ppm2    4 533
ASSI { 4862}
  (( segid "BrD " and resid 104  and name HE1 ))
  (( segid "BrD " and resid 104  and name HD1 ))
   1.900    0 900    0.900 peak  4862 weight  0 11000E+01 volume  0 17529E+04 ppm1    3 571 ppm2    2 290
ASSI { 4912}
  (( segid "BrD " and resid 57   and name HG1 ))
  (( segid "BrD " and resid 57   and name HA  ))
   2 400    1 400    1 400 peak  4912 weight  0 11000E+01 volume  0 42230E+03 ppm1    2.110 ppm2    4 800
ASSI { 4922}
  (( segid "BrD " and resid 97   and name HE1 ))
  (( segid "BrD " and resid 97   and name HG2 ))
   2 200    1 200    1 200 peak  4922 weight  0 11000E+01 volume  0 69710E+03 ppm1    3.569 ppm2    2 172
ASSI { 4932}
  (( segid "BrD " and resid 109  and name HA  ))
  (( segid "BrD " and resid 109  and name HB2 ))
   2 000    1.000    1 000 peak  4932 weight  0 11000E+01 volume  0 10760E+04 ppm1    4.653 ppm2    2 149
ASSI { 4942}
  (( segid "BrD " and resid 109  and name HA  ))
  (( segid "BrD " and resid 109  and name HB1 ))
   2.000    1 000    1 000 peak  4942 weight  0 11000E+01 volume  0 13416E+04 ppm1    4 653 ppm2    2.321
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ASSI { 4962}
  (( segid "BrD " and resid 109  and name HB2 ))
  (( segid "BrD " and resid 109  and name HG1 ))
   2 500     1 600     1 600 peak  4962 weight  0 11000E+01 volume  0 29632E+03 ppm1      2 141 ppm2      1 417
ASSI { 4972}
  (( segid "BrD " and resid 109  and name HB1 ))
  (( segid "BrD " and resid 109  and name HG1 ))
   2 500     1 600     1 600 peak  4972 weight  0.11000E+01 volume  0 36408E+03 ppm1      2 334 ppm2      1 417
ASSI { 4982}
  (( segid "BrD " and resid 109  and name HG1 ))
  (( segid "BrD " and resid 109  and name HA  ))
   2 700     1 800     1 800 peak  4982 weight  0 11000E+01 volume  0 22259E+03 ppm1      1 399 ppm2      4 639
ASSI { 5002}
  (( segid "BrD " and resid 109  and name HB2 ))
  (( segid "BrD " and resid 109  and name HA  ))
   2 800     2 000     2 000 peak  5002 weight  0.11000E+01 volume  0 16510E+03 ppm1      3 029 ppm2      4 639
ASSI { 5012}
  (( segid "BrD " and resid 86   and name HG2 ))
  (( segid "BrD " and resid 86   and name HA  ))
   2 800     2.000     2 000 peak  5012 weight  0 11000E+01 volume  0 18063E+03 ppm1      0 761 ppm2      4 812
ASSI { 5022}
  (  segid "BrD " and resid 41   and name HG2%)
  (( segid "BrD " and resid 41   and name HA  ))
   2 200     1 200     1.200 peak  5022 weight  0 11000E+01 volume  0 76022E+03 ppm1      1 844 ppm2      4 671
ASSI { 5032}
  (  segid "BrD " and resid 41   and name HG2%)
  (( segid "BrD " and resid 41   and name HB  ))
   2 000     1 000     1 000 peak  5032 weight  0.11000E+01 volume  0 12138E+04 ppm1      1 845 ppm2      4 901
ASSI { 5042}
  (  segid "BrD " and resid 58   and name HG2%)
  (( segid "BrD " and resid 58   and name HA  ))
   2 000     1 000     1 000 peak  5042 weight  0 11000E+01 volume  0 10840E+04 ppm1      1 649 ppm2      4 451
ASSI { 5052}
  (  segid "BrD " and resid 58   and name HG2%)
  (( segid "BrD " and resid 58   and name HB  ))
   1 900     0 900     0 900 peak  5052 weight  0 11000E+01 volume  0 14547E+04 ppm1      1 649 ppm2      4 705
ASSI { 5062}
  (  segid "BrD " and resid 17   and name HG2%)
  (( segid "BrD " and resid 17   and name HA  ))
   2 300     1 300     1 300 peak  5062 weight  0 11000E+01 volume  0 54601E+03 ppm1      1 747 ppm2      4 542
ASSI { 5072}
  (  segid "BrD " and resid 17   and name HG2%)
  (( segid "BrD " and resid 17   and name HB  ))
   2 100     1 100     1 100 peak  5072 weight  0 11000E+01 volume  0 92706E+03 ppm1      1 745 ppm2      4 861
ASSI { 5082}
  (  segid "BrD " and resid 83   and name HG2%)
  (( segid "BrD " and resid 83   and name HB  ))
   2 100     1 100     1 100 peak  5082 weight  0 11000E+01 volume  0 10099E+04 ppm1      1 893 ppm2      4 805
ASSI { 5092}
  (  segid "BrD " and resid 83   and name HG2%)
  (( segid "BrD " and resid 83   and name HA  ))
   2 200     1 200     1.200 peak  5092 weight  0 11000E+01 volume  0 64890E+03 ppm1      1 894 ppm2      4 460
ASSI { 5122}
  (( segid "BrD " and resid 37   and name HA  ))
  (( segid "BrD " and resid 37   and name HG1 ))
   2 800     2 000     2 000 peak  5122 weight  0 11000E+01 volume  0 14935E+03 ppm1      4.853 ppm2      2 725
ASSI { 5132}
  (( segid "BrD " and resid 37   and name HA  ))
  (( segid "BrD " and resid 37   and name HG2 ))
   3 200     2.600     2.300 peak  5132 weight  0 11000E+01 volume  0 80336E+02 ppm1      4 853 ppm2      2 587
ASSI { 5162}
  (( segid "BrD " and resid 37   and name HG2 ))
  (( segid "BrD " and resid 37   and name HD1 ))
   2 300     1 300     1 300 peak  5162 weight  0.11000E+01 volume  0 49428E+03 ppm1      2 585 ppm2      4 291
ASSI { 5172}
  (( segid "BrD " and resid 37   and name HG1 ))
  (( segid "BrD " and resid 37   and name HD1 ))
   2 500     1 600     1 600 peak  5172 weight  0 11000E+01 volume  0 34945E+03 ppm1      2 733 ppm2      4 290
ASSI { 5182}
  (( segid "BrD " and resid 37   and name HG1 ))
  (( segid "BrD " and resid 37   and name HB1 ))
   2.300     1 300     1 300 peak  5182 weight  0 11000E+01 volume  0 51291E+03 ppm1      2 733 ppm2      2 961
ASSI { 5192}
  (( segid "BrD " and resid 37   and name HG2 ))
  (( segid "BrD " and resid 37   and name HB1 ))
   2 300     1 300     1 300 peak  5192 weight  0 11000E+01 volume  0 56233E+03 ppm1      2 584 ppm2      2 961
ASSI { 5202}
  (( segid "BrD " and resid 37   and name HB1 ))
  (( segid "BrD " and resid 37   and name HA  ))
   2 200     1 200     1 200 peak  5202 weight  0 11000E+01 volume  0 64791E+03 ppm1      2 935 ppm2      4 858
ASSI { 5212}
  (( segid "BrD " and resid 37   and name HB2 ))
  (( segid "BrD " and resid 37   and name HA  ))
   2 400     1 400     1 400 peak  5212 weight  0 11000E+01 volume  0 38926E+03 ppm1      2 290 ppm2      4 858
ASSI { 5222}
  (( segid "BrD " and resid 37   and name HB1 ))
  (( segid "BrD " and resid 37   and name HD1 ))
   3 600     3 200     1 900 peak  5222 weight  0 11000E+01 volume  0 35025E+02 ppm1      2 935 ppm2      4 298
ASSI { 5272}
  (( segid "BrD " and resid 53   and name HD1 ))
  (( segid "BrD " and resid 52   and name HA  ))
   3 300     2 700     2 200 peak  5272 weight  0 11000E+01 volume  0 65454E+02 ppm1      4 214 ppm2      5 584
ASSI { 5282}
  (( segid "BrD " and resid 53   and name HB1 ))
  (( segid "BrD " and resid 53   and name HA  ))
   2 200     1 200     1 200 peak  5282 weight  0 11000E+01 volume  0.77735E+03 ppm1      2 780 ppm2      4 686
ASSI { 5292}
  (( segid "BrD " and resid 53   and name HG2 ))
  (( segid "BrD " and resid 53   and name HA  ))
   2 900     2 100     2 100 peak  5292 weight  0.11000E+01 volume  0 13443E+03 ppm1      2.487 ppm2      4 687
ASSI { 5302}
  (( segid "BrD " and resid 51   and name HA  ))
  (( segid "BrD " and resid 51   and name HG2 ))
   2 300     1 300     1 300 peak  5302 weight  0 11000E+01 volume  0 54723E+03 ppm1      4 459 ppm2      1 796
ASSI { 5312}
  (( segid "BrD " and resid 51   and name HA  ))
  (( segid "BrD " and resid 51   and name HG1 ))
   2 400     1 400     1 400 peak  5312 weight  0 11000E+01 volume  0 38819E+03 ppm1      4 459 ppm2      1 946
ASSI { 5332}
  (( segid "BrD " and resid 51   and name HB1 ))
  (( segid "BrD " and resid 51   and name HA  ))
   2.700     1 800     1 800 peak  5332 weight  0 11000E+01 volume  0 20757E+03 ppm1      1 945 ppm2      4 468
ASSI { 5342}
  (( segid "BrD " and resid 51   and name HB2 ))
  (( segid "BrD " and resid 51   and name HA  ))
   2 400     1 400     1 400 peak  5342 weight  0.11000E+01 volume  0 37628E+03 ppm1      1.795 ppm2      4 468
ASSI { 5372}
  (( segid "BrD " and resid 51   and name HG1 ))
  (( segid "BrD " and resid 51   and name HD1 ))
   2 800     2 000     2 000 peak  5372 weight  0 11000E+01 volume  0.16452E+03 ppm1      1 946 ppm2      3 606
ASSI { 5382}
  (( segid "BrD " and resid 51   and name HG2 ))
  (( segid "BrD " and resid 51   and name HD1 ))
   2 400     1 400     1 400 peak  5382 weight  0.11000E+01 volume  0 40668E+03 ppm1      1 796 ppm2      3 606
ASSI { 5392}
  (( segid "BrD " and resid 51   and name HD1 ))
  (( segid "BrD " and resid 51   and name HB1 ))
   2 500     1 600     1 600 peak  5392 weight  0 11000E+01 volume  0 36659E+03 ppm1      3 577 ppm2      1 945
ASSI { 5402}
  (( segid "BrD " and resid 51   and name HD1 ))
  (( segid "BrD " and resid 51   and name HB2 ))
   2 400     1 400     1 400 peak  5402 weight  0 11000E+01 volume  0 38417E+03 ppm1      3 577 ppm2      1 795
ASSI { 5412}
  (( segid "BrD " and resid 51   and name HD1 ))
  (( segid "BrD " and resid 51   and name HA  ))
   2 700     1 800     1 800 peak  5412 weight  0 11000E+01 volume  0 20141E+03 ppm1      3 578 ppm2      4 463
ASSI { 5422}
  (( segid "BrD " and resid 52   and name HA  ))
  (( segid "BrD " and resid 52   and name HB1 ))
   2 500     1 600     1 600 peak  5422 weight  0 11000E+01 volume  0.31370E+03 ppm1      5 592 ppm2      3 654
ASSI { 5432}
  (( segid "BrD " and resid 52   and name HA  ))
  (( segid "BrD " and resid 52   and name HB2 ))
   2 800     2 000     2 000 peak  5432 weight  0 11000E+01 volume  0 16779E+03 ppm1      5 592 ppm2      3 533
ASSI { 5462}
  (( segid "BrD " and resid 75   and name HG2 ))
  (( segid "BrD " and resid 75   and name HA  ))
   2.700     1 800     1 800 peak  5462 weight  0 11000E+01 volume  0 19830E+03 ppm1      3 228 ppm2      4 517
ASSI { 5482}
  (( segid "BrD " and resid 75   and name HG2 ))
  (( segid "BrD " and resid 75   and name HB2 ))
   2 600     1 700     1 700 peak  5482 weight  0 11000E+01 volume  0 27353E+03 ppm1      3 227 ppm2      2 847
ASSI { 5492}
  (( segid "BrD " and resid 75   and name HG1 ))
  (( segid "BrD " and resid 75   and name HB2 ))
   2 300     1 300     1 300 peak  5492 weight  0 11000E+01 volume  0 48028E+03 ppm1      3 523 ppm2      2.847
ASSI { 5502}
  (( segid "BrD " and resid 75   and name HG1 ))
  (( segid "BrD " and resid 75   and name HB1 ))
   2 700     1 800     1 800 peak  5502 weight  0 11000E+01 volume  0.21586E+03 ppm1      3 523 ppm2      2 931
ASSI { 5512}
  (( segid "BrD " and resid 75   and name HG2 ))
  (( segid "BrD " and resid 75   and name HB1 ))
   2 700     1 800     1 800 peak  5512 weight  0 11000E+01 volume  0 21836E+03 ppm1      3 227 ppm2      2.931
ASSI { 5522}
  (( segid "BrD " and resid 75   and name HA  ))
  (( segid "BrD " and resid 75   and name HG1 ))
   2 800     2 000     2 000 peak  5522 weight  0 11000E+01 volume  0 16121E+03 ppm1      4 509 ppm2      3 530
ASSI { 5542}
  (( segid "BrD " and resid 19   and name HB2 ))
  (( segid "BrD " and resid 16   and name HA  ))
   2.900     2 100     2.100 peak  5542 weight  0 11000E+01 volume  0 12463E+03 ppm1      1.989 ppm2      4 507
ASSI { 5552}
  (( segid "BrD " and resid 19   and name HB2 ))
  (( segid "BrD " and resid 19   and name HA  ))
   2 600     1 700     1 700 peak  5552 weight  0 11000E+01 volume  0.27005E+03 ppm1      1 989 ppm2      4 297
ASSI { 5582}
  (( segid "BrD " and resid 54   and name HA  ))
  (( segid "BrD " and resid 54   and name HB2 ))
   3 000     2.200     2 200 peak  5582 weight  0 11000E+01 volume  0.10290E+03 ppm1      5 543 ppm2      1 964
ASSI { 5592}
  (( segid "BrD " and resid 97   and name HG1 ))
  (( segid "BrD " and resid 97   and name HE1 ))
   3.100     2 400     2 400 peak  5592 weight  0 11000E+01 volume  0 89029E+02 ppm1      2.436 ppm2      3 572
ASSI { 5622}
  (( segid "BrD " and resid 59   and name HG2 ))
  (( segid "BrD " and resid 59   and name HA  ))
   2.400     1 400     1 400 peak  5622 weight  0 11000E+01 volume  0 39102E+03 ppm1      3.137 ppm2      4 911
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ASSI { 5632}
   (( segid "BrD " and resid 59   and name HG1 ))
   (( segid "BrD " and resid 59   and name HA  ))
     3 000     2.200     2 200 peak  5632 weight  0.11000E+01 volume  0 11482E+03 ppm1      3 228 ppm2      4 911
ASSI { 5642}
   (( segid "BrD " and resid 13   and name HG2 ))
   (( segid "BrD " and resid 13   and name HA  ))
     2 300     1 300     1 300 peak  5642 weight  0.11000E+01 volume  0.56353E+03 ppm1      2 978 ppm2      4 775
ASSI { 5652}
   (( segid "BrD " and resid 13   and name HG1 ))
   (( segid "BrD " and resid 13   and name HA  ))
     2 800     2 000     2.000 peak  5652 weight  0 11000E+01 volume  0 18150E+03 ppm1      3 131 ppm2      4 775
ASSI { 5672}
   (( segid "BrD " and resid 57   and name HA  ))
   (( segid "BrD " and resid 57   and name HD1 ))
     2 600     1 700     1 700 peak  5672 weight  0 11000E+01 volume  0 27608E+03 ppm1      4 805 ppm2      2 387
ASSI { 5682}
   (( segid "BrD " and resid 57   and name HA  ))
   (( segid "BrD " and resid 57   and name HG2 ))
     2 900     2 100     2 100 peak  5682 weight  0.11000E+01 volume  0 12195E+03 ppm1      4 805 ppm2      2 016
ASSI { 5712}
   (( segid "BrD " and resid 57   and name HB2 ))
   (( segid "BrD " and resid 57   and name HA  ))
     2 500     1 600     1 600 peak  5712 weight  0 11000E+01 volume  0 35277E+03 ppm1      2 843 ppm2      4 800
ASSI { 5722}
   (( segid "BrD " and resid 57   and name HB1 ))
   (( segid "BrD " and resid 57   and name HA  ))
     2 400     1 400     1.400 peak  5722 weight  0 11000E+01 volume  0 42344E+03 ppm1      2 935 ppm2      4 798
ASSI { 5732}
   (( segid "BrD " and resid 57   and name HE1 ))
   (( segid "BrD " and resid 57   and name HG2 ))
     2 200     1 200     1 200 peak  5732 weight  0 11000E+01 volume  0 67766E+03 ppm1      3 572 ppm2      2 017
ASSI { 5752}
   (( segid "BrD " and resid 57   and name HD2 ))
   (( segid "BrD " and resid 57   and name HA  ))
     2 600     1 700     1 700 peak  5752 weight  0 11000E+01 volume  0 24171E+03 ppm1      2 295 ppm2      4 800
ASSI { 5762}
   (( segid "BrD " and resid 57   and name HD1 ))
   (( segid "BrD " and resid 57   and name HE1 ))
     2 100     1 100     1 100 peak  5762 weight  0 11000E+01 volume  0 83932E+03 ppm1      2 387 ppm2      3 591
ASSI { 5772}
   (( segid "BrD " and resid 57   and name HD2 ))
   (( segid "BrD " and resid 57   and name HE1 ))
     2 100     1 100     1 100 peak  5772 weight  0 11000E+01 volume  0 96087E+03 ppm1      2 289 ppm2      3 591
ASSI { 5792}
   (( segid "BrD " and resid 12   and name HA  ))
   (( segid "BrD " and resid 12   and name HB2 ))
     2 700     1 800     1 800 peak  5792 weight  0 11000E+01 volume  0.22035E+03 ppm1      5 297 ppm2      3 338
ASSI { 5812}
   (( segid "BrD " and resid 57   and name HG1 ))
   (( segid "BrD " and resid 57   and name HE1 ))
     2 600     1 700     1 700 peak  5812 weight  0 11000E+01 volume  0 23002E+03 ppm1      2 099 ppm2      3 590
ASSI { 5822}
   (( segid "BrD " and resid 26   and name HA  ))
   (( segid "BrD " and resid 26   and name HB1 ))
     2 100     1 100     1 100 peak  5822 weight  0 11000E+01 volume  0 10358E+04 ppm1      4 509 ppm2      2 482
ASSI { 5832}
   (( segid "BrD " and resid 26   and name HA  ))
   (( segid "BrD " and resid 26   and name HD1 ))
     2 700     1 800     1 800 peak  5832 weight  0.11000E+01 volume  0 18918E+03 ppm1      4 509 ppm2      2 109
ASSI { 5842}
   (( segid "BrD " and resid 26   and name HA  ))
   (( segid "BrD " and resid 26   and name HG1 ))
     3 200     2 600     2 300 peak  5842 weight  0.11000E+01 volume  0 75991E+02 ppm1      4 509 ppm2      1 629
ASSI { 5852}
   (( segid "BrD " and resid 10   and name HA  ))
   (( segid "BrD " and resid 10   and name HB2 ))
     2 800     2 000     2 000 peak  5852 weight  0 11000E+01 volume  0 18381E+03 ppm1      5 478 ppm2      3 300
ASSI { 5862}
   (( segid "BrD " and resid 56   and name HA  ))
   (( segid "BrD " and resid 56   and name HB2 ))
     2 800     2 000     2 000 peak  5862 weight  0 11000E+01 volume  0 18369E+03 ppm1      4 607 ppm2      2 003
ASSI { 5872}
   (  segid "BrD " and resid 56   and name HD2%)
   (( segid "BrD " and resid 56   and name HB2 ))
     2 600     1.700     1 700 peak  5872 weight  0 11000E+01 volume  0 24752E+03 ppm1      1.254 ppm2      2.004
ASSI { 5882}
   (  segid "BrD " and resid 69   and name HG1%)
   (( segid "BrD " and resid 69   and name HB  ))
     2.100     1.100     1 100 peak  5882 weight  0 11000E+01 volume  0 96122E+03 ppm1      1 548 ppm2      2 922
ASSI { 5892}
   (  segid "BrD " and resid 69   and name HG2%)
   (( segid "BrD " and resid 69   and name HB  ))
     2 100     1.100     1 100 peak  5892 weight  0 11000E+01 volume  0 91489E+03 ppm1      1 424 ppm2      2 919
ASSI { 5902}
   (  segid "BrD " and resid 69   and name HG2%)
   (( segid "BrD " and resid 69   and name HA  ))
     2 600     1 700     1 700 peak  5902 weight  0.11000E+01 volume  0.28227E+03 ppm1      1 425 ppm2      4 696
ASSI { 5912}
   (  segid "BrD " and resid 78   and name HD2%)
   (( segid "BrD " and resid 78   and name HA  ))
     2 800     2 000     2 000 peak  5912 weight  0 11000E+01 volume  0.18293E+03 ppm1      0 662 ppm2      3 999
ASSI { 5922}
   (  segid "BrD " and resid 78   and name HD2%)
   (( segid "BrD " and resid 78   and name HB2 ))
     2 600     1 700     1 700 peak  5922 weight  0 11000E+01 volume  0 24706E+03 ppm1      0 662 ppm2      1 039
ASSI { 5932}
   (  segid "BrD " and resid 78   and name HD2%)
   (( segid "BrD " and resid 78   and name HG  ))
     2 300     1 300     1 300 peak  5932 weight  0 11000E+01 volume  0 60283E+03 ppm1      0 662 ppm2      1 270
ASSI { 5962}
   (( segid "BrD " and resid 18   and name HA  ))
   (  segid "BrD " and resid 18   and name HD1%)
     2 600     1 700     1 700 peak  5962 weight  0 11000E+01 volume  0 27810E+03 ppm1      3 867 ppm2      1 079
ASSI { 5982}
   (  segid "BrD " and resid 18   and name HD1%)
   (( segid "BrD " and resid 18   and name HG  ))
     2 700     1 800     1 800 peak  5982 weight  0 11000E+01 volume  0 22916E+03 ppm1      1.057 ppm2      2 278
ASSI { 5992}
   (  segid "BrD " and resid 18   and name HD2%)
   (( segid "BrD " and resid 18   and name HB1 ))
     2 600     1.700     1 700 peak  5992 weight  0 11000E+01 volume  0 25721E+03 ppm1      0 418 ppm2      2 137
ASSI { 6002}
   (( segid "BrD " and resid 102  and name HG  ))
   (  segid "BrD " and resid 102  and name HD1%)
     2.300     1 300     1 300 peak  6002 weight  0 11000E+01 volume  0 47853E+03 ppm1      2.141 ppm2      1 324
ASSI { 6012}
   (( segid "BrD " and resid 73   and name HB1 ))
   (  segid "BrD " and resid 73   and name HD2%)
     2 300     1 300     1 300 peak  6012 weight  0 11000E+01 volume  0 54334E+03 ppm1      2 583 ppm2      1.483
ASSI { 6052}
   (( segid "BrD " and resid 73   and name HA  ))
   (( segid "BrD " and resid 73   and name HB1 ))
     2 400     1 400     1 400 peak  6052 weight  0.11000E+01 volume  0.44904E+03 ppm1      4.805 ppm2      2 594
ASSI { 6072}
   (  segid "BrD " and resid 73   and name HD1%)
   (( segid "BrD " and resid 73   and name HA  ))
     2.500     1.600     1 600 peak  6072 weight  0 11000E+01 volume  0 30560E+03 ppm1      1 549 ppm2      4 825
ASSI { 6112}
   (( segid "BrD " and resid 56   and name HB1 ))
   (  segid "BrD " and resid 56   and name HD1%)
     2 700     1 800     1 800 peak  6112 weight  0 11000E+01 volume  0 20480E+03 ppm1      2.685 ppm2      1 538
ASSI { 6122}
   (( segid "BrD " and resid 56   and name HB2 ))
   (  segid "BrD " and resid 56   and name HD1%)
     2 900     2 100     2 100 peak  6122 weight  0 11000E+01 volume  0 13067E+03 ppm1      1.994 ppm2      1 538
ASSI { 6162}
   (( segid "BrD " and resid 56   and name HG  ))
   (  segid "BrD " and resid 56   and name HD1%)
     2 300     1 300     1 300 peak  6162 weight  0 11000E+01 volume  0 52968E+03 ppm1      2 339 ppm2      1.539
ASSI { 6212}
   (( segid "BrD " and resid 22   and name HA  ))
   (  segid "BrD " and resid 22   and name HD1%)
     2.500     1 600     1 600 peak  6212 weight  0 11000E+01 volume  0 33531E+03 ppm1      4 706 ppm2      1 648
ASSI { 6232}
   (  segid "BrD " and resid 22   and name HD1%)
   (( segid "BrD " and resid 22   and name HB1 ))
     2 400     1 400     1 400 peak  6232 weight  0 11000E+01 volume  0 37274E+03 ppm1      1 648 ppm2      2 702
ASSI { 6242}
   (  segid "BrD " and resid 22   and name HD1%)
   (( segid "BrD " and resid 22   and name HG  ))
     2 200     1 200     1 200 peak  6242 weight  0 11000E+01 volume  0 77165E+03 ppm1      1.648 ppm2      2 361
ASSI { 6272}
   (  segid "BrD " and resid 63   and name HD2%)
   (( segid "BrD " and resid 63   and name HG  ))
     2.600     1 700     1 700 peak  6272 weight  0 11000E+01 volume  0 24631E+03 ppm1      1 498 ppm2      2 424
ASSI { 6282}
   (  segid "BrD " and resid 63   and name HD1%)
   (( segid "BrD " and resid 63   and name HG  ))
     2 700     1 800     1 800 peak  6282 weight  0 11000E+01 volume  0 21403E+03 ppm1      1.649 ppm2      2 424
ASSI { 6322}
   (( segid "BrD " and resid 66   and name HG2 ))
   (( segid "BrD " and resid 66   and name HD2 ))
     2 500     1 600     1 600 peak  6322 weight  0 11000E+01 volume  0 35570E+03 ppm1      2 140 ppm2      3 637
ASSI { 6352}
   (( segid "BrD " and resid 66   and name HD2 ))
   (( segid "BrD " and resid 66   and name HA  ))
     2.500     1 600     1 600 peak  6352 weight  0 11000E+01 volume  0 30900E+03 ppm1      3 631 ppm2      4.998
ASSI { 6392}
   (( segid "BrD " and resid 100  and name HB1 ))
   (( segid "BrD " and resid 100  and name HA  ))
     2 100     1.100     1 100 peak  6392 weight  0 11000E+01 volume  0 94220E+03 ppm1      3 455 ppm2      4 949
ASSI { 6412}
   (( segid "BrD " and resid 114  and name HA1 ))
   (( segid "BrD " and resid 114  and name HA2 ))
     2 100     1 100     1 100 peak  6412 weight  0 11000E+01 volume  0.97579E+03 ppm1      4 600 ppm2      4 522
ASSI { 6432}
   (( segid "BrD " and resid 85   and name HA  ))
   (( segid "BrD " and resid 85   and name HB1 ))
     2.700     1 800     1 800 peak  6432 weight  0 11000E+01 volume  0.21987E+03 ppm1      5 001 ppm2      3 906
ASSI { 6442}
   (( segid "BrD " and resid 85   and name HA  ))
   (( segid "BrD " and resid 85   and name HB2 ))
     2 800     2 000     2 000 peak  6442 weight  0 11000E+01 volume  0 16015E+03 ppm1      5.000 ppm2      3 621
ASSI { 6492}
   (( segid "BrD " and resid 98   and name HA  ))
   (( segid "BrD " and resid 98   and name HB1 ))
     2 800     2.000     2 000 peak  6492 weight  0 11000E+01 volume  0 16821E+03 ppm1      4 804 ppm2      4 014
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ASSI { 6502}
  (( segid "BrD " and resid 98   and name HA  ))
  (( segid "BrD " and resid 98   and name HB2 ))
    2 700     1 800     1 800 peak  6502 weight  0 11000E+01 volume  0.19206E+03 ppm1     4 804 ppm2     3 660
ASSI { 6512}
  (( segid "BrD " and resid 32   and name HA  ))
  (( segid "BrD " and resid 32   and name HB2 ))
    2 700     1 800     1 800 peak  6512 weight  0 11000E+01 volume  0 22946E+03 ppm1     4 953 ppm2     3 965
ASSI { 6522}
  (( segid "BrD " and resid 32   and name HA  ))
  (( segid "BrD " and resid 32   and name HB1 ))
    2 700     1 800     1 800 peak  6522 weight  0 11000E+01 volume  0 20617E+03 ppm1     4.954 ppm2     4 206
ASSI { 6552}
  (( segid "BrD " and resid 11   and name HA  ))
  (( segid "BrD " and resid 11   and name HG1 ))
    2 600     1 700     1 700 peak  6552 weight  0 11000E+01 volume  0 23807E+03 ppm1     4 951 ppm2     2 635
ASSI { 6562}
  (( segid "BrD " and resid 53   and name HG1 ))
  (( segid "BrD " and resid 53   and name HA  ))
    2.700     1 800     1 800 peak  6562 weight  0 11000E+01 volume  0 20893E+03 ppm1     2 784 ppm2     4 687
ASSI { 6572}
  (( segid "BrD " and resid 31   and name HA  ))
  (  segid "BrD " and resid 102  and name HD1%)
    2 500     1 600     1 600 peak  6572 weight  0.11000E+01 volume  0 36090E+03 ppm1     5 000 ppm2     1 323
ASSI { 6612}
  (  segid "BrD " and resid 31   and name HB% )
  (  segid "BrD " and resid 102  and name HD1%)
    2.500     1 600     1 600 peak  6612 weight  0 11000E+01 volume  0 31261E+03 ppm1     2 289 ppm2     1 320
ASSI { 6642}
  (( segid "BrD " and resid 43   and name HA  ))
  (( segid "BrD " and resid 44   and name HD2 ))
    2.400     1 400     1 400 peak  6642 weight  0 11000E+01 volume  0 39497E+03 ppm1     5 547 ppm2     4.127
ASSI { 6662}
  (  segid "BrD " and resid 43   and name HB% )
  (( segid "BrD " and resid 44   and name HD2 ))
    2 700     1 800     1 800 peak  6662 weight  0 11000E+01 volume  0 20471E+03 ppm1     1 700 ppm2     4.135
ASSI { 6672}
  (  segid "BrD " and resid 43   and name HB% )
  (( segid "BrD " and resid 46   and name HB1 ))
    2.600     1 700     1 700 peak  6672 weight  0 11000E+01 volume  0 27100E+03 ppm1     1 697 ppm2     3 295
ASSI { 6682}
  (  segid "BrD " and resid 43   and name HB% )
  (( segid "BrD " and resid 46   and name HB2 ))
    2.700     1 800     1 800 peak  6682 weight  0 11000E+01 volume  0 19809E+03 ppm1     1 697 ppm2     3 100
ASSI { 6732}
  (( segid "BrD " and resid 76   and name HA  ))
  (( segid "BrD " and resid 79   and name HB1 ))
    2 800     2 000     2 000 peak  6732 weight  0 11000E+01 volume  0 16513E+03 ppm1     4 658 ppm2     2 774
ASSI { 6872}
  (  segid "BrD " and resid 113  and name HB% )
  (  segid "BrD " and resid 17   and name HG2%)
    2 500     1 600     1 600 peak  6872 weight  0 11000E+01 volume  0 31889E+03 ppm1     1 994 ppm2     1 750
ASSI { 6882}
  (( segid "BrD " and resid 79   and name HA  ))
  (( segid "BrD " and resid 79   and name HB1 ))
    2 700     1 800     1 800 peak  6882 weight  0 11000E+01 volume  0 19089E+03 ppm1     4 409 ppm2     2 781
ASSI { 6892}
  (( segid "BrD " and resid 79   and name HA  ))
  (( segid "BrD " and resid 79   and name HB2 ))
    2 200     1 200     1 200 peak  6892 weight  0 11000E+01 volume  0 79324E+03 ppm1     4 409 ppm2     2.678
ASSI { 6912}
  (  segid "BrD " and resid 43   and name HB% )
  (( segid "BrD " and resid 44   and name HD1 ))
    2 900     2 100     2 100 peak  6912 weight  0 11000E+01 volume  0 13650E+03 ppm1     1 700 ppm2     4 337
ASSI { 6942}
  (  segid "BrD " and resid 25   and name HG1%)
  (  segid "BrD " and resid 102  and name HD1%)
    2 700     1 800     1 800 peak  6942 weight  0 11000E+01 volume  0 21235E+03 ppm1     1 795 ppm2     1 323
ASSI { 6962}
  (  segid "BrD " and resid 25   and name HG1%)
  (  segid "BrD " and resid 78   and name HD1%)
    3.000     2 200     2 200 peak  6962 weight  0 11000E+01 volume  0 99662E+02 ppm1     1 798 ppm2     0 774
ASSI { 6972}
  (  segid "BrD " and resid 25   and name HG1%)
  (  segid "BrD " and resid 78   and name HD2%)
    2 800     2 000     2 000 peak  6972 weight  0 11000E+01 volume  0 15213E+03 ppm1     1 797 ppm2     0 673
ASSI { 6992}
  (  segid "BrD " and resid 25   and name HG2%)
  (  segid "BrD " and resid 102  and name HD1%)
    2.200     1 200     1 200 peak  6992 weight  0 11000E+01 volume  0 77265E+03 ppm1     1 646 ppm2     1 324
ASSI { 7002}
  (  segid "BrD " and resid 25   and name HG2%)
  (  segid "BrD " and resid 78   and name HD1%)
    2.800     2 000     2 000 peak  7002 weight  0 11000E+01 volume  0 16697E+03 ppm1     1 646 ppm2     0 775
ASSI { 7022}
  (( segid "BrD " and resid 38   and name HB  ))
  (( segid "BrD " and resid 38   and name HA  ))
    2.800     2 000     2 000 peak  7022 weight  0 11000E+01 volume  0 17527E+03 ppm1     1 751 ppm2     4 170
ASSI { 7032}
  (  segid "BrD " and resid 38   and name HG2%)
  (  segid "BrD " and resid 43   and name HB% )
    2 200     1 200     1 200 peak  7032 weight  0 11000E+01 volume  0 74974E+03 ppm1     0 808 ppm2     1 715
ASSI { 7092}
  (( segid "BrD " and resid 81   and name HA  ))
  (( segid "BrD " and resid 81   and name HB  ))
    2 800     2 000     2 000 peak  7092 weight  0.11000E+01 volume  0 15198E+03 ppm1     3.718 ppm2     2 037
ASSI { 7102}
  (( segid "BrD " and resid 81   and name HB  ))
  (( segid "BrD " and resid 78   and name HA  ))
    3 100     2 400     2 400 peak  7102 weight  0 11000E+01 volume  0 98817E+02 ppm1     2 042 ppm2     4 000
ASSI { 7122}
  (  segid "BrD " and resid 81   and name HG1%)
  (( segid "BrD " and resid 78   and name HA  ))
    2 600     1 700     1.700 peak  7122 weight  0 11000E+01 volume  0 25254E+03 ppm1     1.059 ppm2     3 999
ASSI { 7172}
  (  segid "BrD " and resid 81   and name HG2%)
  (( segid "BrD " and resid 34   and name HB1 ))
    2.600     1 700     1 700 peak  7172 weight  0 11000E+01 volume  0 27152E+03 ppm1     0.755 ppm2     4.106
ASSI { 7192}
  (( segid "BrD " and resid 17   and name HA  ))
  (( segid "BrD " and resid 20   and name HB1 ))
    3 200     2 600     2 300 peak  7192 weight  0 11000E+01 volume  0 76028E+02 ppm1     4 542 ppm2     4 671
ASSI { 7252}
  (  segid "BrD " and resid 17   and name HG2%)
  (  segid "BrD " and resid 102  and name HD2%)
    5 500     5 500     0 000 peak  7252 weight  0 11000E+01 volume  0 56051E+00 ppm1     1 745 ppm2     1 320
ASSI { 7272}
  (  segid "BrD " and resid 17   and name HG2%)
  (  segid "BrD " and resid 18   and name HD2%)
    2 800     2 000     2 000 peak  7272 weight  0 11000E+01 volume  0 14970E+03 ppm1     1 747 ppm2     0 409
ASSI { 7352}
  (  segid "BrD " and resid 58   and name HG2%)
  (  segid "BrD " and resid 54   and name HE% )
    2 400     1.400     1 400 peak  7352 weight  0 11000E+01 volume  0 41514E+03 ppm1     1 649 ppm2     2 563
ASSI { 7482}
  (( segid "BrD " and resid 32   and name HA  ))
  (( segid "BrD " and resid 35   and name HG1 ))
    2 900     2 100     2 100 peak  7482 weight  0 11000E+01 volume  0 12205E+03 ppm1     4 953 ppm2     3 451
ASSI { 7492}
  (( segid "BrD " and resid 32   and name HA  ))
  (( segid "BrD " and resid 33   and name HD1 ))
    2.900     2 100     2 100 peak  7492 weight  0 11000E+01 volume  0 14430E+03 ppm1     4.952 ppm2     2 776
ASSI { 7502}
  (( segid "BrD " and resid 62   and name HA  ))
  (( segid "BrD " and resid 62   and name HB1 ))
    2.700     1 800     1 800 peak  7502 weight  0 11000E+01 volume  0 21435E+03 ppm1     4 457 ppm2     2 657
ASSI { 7522}
  (( segid "BrD " and resid 62   and name HA  ))
  (( segid "BrD " and resid 62   and name HG2 ))
    2 800     2 000     2 000 peak  7522 weight  0 11000E+01 volume  0 15009E+03 ppm1     4.457 ppm2     1 478
ASSI { 7532}
  (( segid "BrD " and resid 62   and name HA  ))
  (( segid "BrD " and resid 62   and name HB2 ))
    3 000     2.200     2 200 peak  7532 weight  0 11000E+01 volume  0 10361E+03 ppm1     4 457 ppm2     1 681
ASSI { 7652}
  (( segid "BrD " and resid 74   and name HA  ))
  (  segid "BrD " and resid 59   and name HE% )
    3 100     2 400     2 400 peak  7652 weight  0 11000E+01 volume  0 93787E+02 ppm1     4 361 ppm2     1 879
ASSI { 7662}
  (( segid "BrD " and resid 74   and name HB1 ))
  (( segid "BrD " and resid 71   and name HA  ))
    3 100     2 400     2.400 peak  7662 weight  0 11000E+01 volume  0 98803E+02 ppm1     3 576 ppm2     4 627
ASSI { 7722}
  (( segid "BrD " and resid 105  and name HA  ))
  (( segid "BrD " and resid 108  and name HB1 ))
    3 100     2 400     2 400 peak  7722 weight  0 11000E+01 volume  0 93160E+02 ppm1     4 902 ppm2     4 582
ASSI { 7752}
  (( segid "BrD " and resid 107  and name HA  ))
  (( segid "BrD " and resid 110  and name HB  ))
    2 800     2.000     2 000 peak  7752 weight  0.11000E+01 volume  0 15544E+03 ppm1     4.410 ppm2     2 360
ASSI { 7762}
  (( segid "BrD " and resid 96   and name HA  ))
  (  segid "BrD " and resid 99   and name HB% )
    3.400     2 900     2 100 peak  7762 weight  0 11000E+01 volume  0 54211E+02 ppm1     4 409 ppm2     2 206
ASSI { 7772}
  (( segid "BrD " and resid 107  and name HA  ))
  (( segid "BrD " and resid 110  and name HG11))
    3 100     2 400     2 400 peak  7772 weight  0 11000E+01 volume  0 86608E+02 ppm1     4 408 ppm2     1 715
ASSI { 7782}
  (( segid "BrD " and resid 107  and name HA  ))
  (( segid "BrD " and resid 110  and name HG12))
    2 900     2.100     2 100 peak  7782 weight  0 11000E+01 volume  0 14800E+03 ppm1     4 408 ppm2     1 661
ASSI { 7792}
  (( segid "BrD " and resid 107  and name HA  ))
  (  segid "BrD " and resid 110  and name HG2%)
    3 100     2 400     2 400 peak  7792 weight  0 11000E+01 volume  0.86153E+02 ppm1     4.408 ppm2     1 261
ASSI { 7802}
  (( segid "BrD " and resid 107  and name HA  ))
  (  segid "BrD " and resid 110  and name HD1%)
    3 000     2 200     2.200 peak  7802 weight  0.11000E+01 volume  0.11960E+03 ppm1     4 408 ppm2     1 141
ASSI { 7872}
  (( segid "BrD " and resid 89   and name HA  ))
  (( segid "BrD " and resid 91   and name HD2 ))
    2 700     1.800     1 800 peak  7872 weight  0.11000E+01 volume  0 22343E+03 ppm1     5 641 ppm2     4.407
ASSI { 7892}
  (( segid "BrD " and resid 100  and name HA  ))
  (( segid "BrD " and resid 103  and name HB2 ))
    2 900     2.100     2 100 peak  7892 weight  0 11000E+01 volume  0 12930E+03 ppm1     4 952 ppm2     1.897
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ASSI { 7922}
   (( segid "BrD " and resid 100  and name HB1 ))
   (( segid "BrD " and resid 97   and name HA  ))
     2 600     1 700     1.700 peak  7922 weight  0 11000E+01 volume  0 24354E+03 ppm1     3 455 ppm2     4 798
ASSI { 7932}
   (( segid "BrD " and resid 100  and name HB2 ))
   (( segid "BrD " and resid 97   and name HA  ))
     2 600     1 700     1 700 peak  7932 weight  0 11000E+01 volume  0 23409E+03 ppm1     3 424 ppm2     4 799
ASSI { 7962}
   (( segid "BrD " and resid 12   and name HA  ))
   (( segid "BrD " and resid 15   and name HB2 ))
     2 900     2 100     2 100 peak  7962 weight  0 11000E+01 volume  0 12451E+03 ppm1     5 298 ppm2     3 646
ASSI { 7972}
   (( segid "BrD " and resid 12   and name HA  ))
   (( segid "BrD " and resid 15   and name HB1 ))
     3 100     2 400     2 400 peak  7972 weight  0 11000E+01 volume  0 81954E+02 ppm1     5 297 ppm2     3 812
ASSI { 8032}
   (( segid "BrD " and resid 77   and name HA  ))
   (( segid "BrD " and resid 80   and name HG1 ))
     3 000     2 200     2 200 peak  8032 weight  0 11000E+01 volume  0 10885E+03 ppm1     4 952 ppm2     2 347
ASSI { 8062}
   (( segid "BrD " and resid 85   and name HB2 ))
   (( segid "BrD " and resid 82   and name HA  ))
     3 000     2 200     2 200 peak  8062 weight  0 11000E+01 volume  0 10120E+03 ppm1     3 621 ppm2     4 753
ASSI { 8072}
   (( segid "BrD " and resid 98   and name HB2 ))
   (( segid "BrD " and resid 95   and name HA  ))
     3 100     2 400     2.400 peak  8072 weight  0 11000E+01 volume  0 94016E+02 ppm1     3 667 ppm2     4 447
ASSI { 8102}
   (( segid "BrD " and resid 63   and name HB1 ))
   (( segid "BrD " and resid 60   and name HA  ))
     2 600     1 700     1 700 peak  8102 weight  0 11000E+01 volume  0 27762E+03 ppm1     2 883 ppm2     4 808
ASSI { 8112}
   (( segid "BrD " and resid 63   and name HB2 ))
   (( segid "BrD " and resid 60   and name HA  ))
     2 700     1 800     1 800 peak  8112 weight  0 11000E+01 volume  0 20887E+03 ppm1     2 538 ppm2     4 809
ASSI { 8142}
   (  segid "BrD " and resid 63   and name HD1%)
   (( segid "BrD " and resid 18   and name HB2 ))
     2 800     2 000     2 000 peak  8142 weight  0.11000E+01 volume  0 16157E+03 ppm1     1 649 ppm2     0 919
ASSI { 8152}
   (  segid "BrD " and resid 63   and name HD1%)
   (  segid "BrD " and resid 18   and name HD1%)
     2 700     1 800     1 800 peak  8152 weight  0 11000E+01 volume  0 20633E+03 ppm1     1 646 ppm2     1 085
ASSI { 8162}
   (  segid "BrD " and resid 63   and name HD1%)
   (( segid "BrD " and resid 18   and name HB1 ))
     2 400     1 400     1 400 peak  8162 weight  0 11000E+01 volume  0 38153E+03 ppm1     1 649 ppm2     2 139
ASSI { 8172}
   (  segid "BrD " and resid 63   and name HD2%)
   (( segid "BrD " and resid 19   and name HA  ))
     2 400     1 400     1 400 peak  8172 weight  0 11000E+01 volume  0 45741E+03 ppm1     1 501 ppm2     4 295
ASSI { 8182}
   (( segid "BrD " and resid 14   and name HB2 ))
   (( segid "BrD " and resid 14   and name HG  ))
     3 100     2 400     2 400 peak  8182 weight  0 11000E+01 volume  0 92156E+02 ppm1     2 145 ppm2     2 059
ASSI { 8192}
   (( segid "BrD " and resid 14   and name HB1 ))
   (( segid "BrD " and resid 14   and name HG  ))
     2 600     1 700     1 700 peak  8192 weight  0 11000E+01 volume  0 23309E+03 ppm1     2 444 ppm2     2 059
ASSI { 8222}
   (  segid "BrD " and resid 14   and name HD2%)
   (  segid "BrD " and resid 18   and name HD2%)
     2 500     1 600     1 600 peak  8222 weight  0 11000E+01 volume  0 31711E+03 ppm1     1 401 ppm2     0 409
ASSI { 8232}
   (  segid "BrD " and resid 14   and name HD2%)
   (  segid "BrD " and resid 18   and name HD1%)
     2 400     1 400     1 400 peak  8232 weight  0 11000E+01 volume  0 46026E+03 ppm1     1.401 ppm2     1 085
ASSI { 8302}
   (( segid "BrD " and resid 18   and name HA  ))
   (( segid "BrD " and resid 18   and name HB2 ))
     2 700     1 800     1 800 peak  8302 weight  0 11000E+01 volume  0 20320E+03 ppm1     3 867 ppm2     0 920
ASSI { 8392}
   (  segid "BrD " and resid 18   and name HD1%)
   (( segid "BrD " and resid 18   and name HB2 ))
     2 400     1 400     1.400 peak  8392 weight  0 11000E+01 volume  0.39910E+03 ppm1     1 057 ppm2     0 925
ASSI { 8402}
   (  segid "BrD " and resid 18   and name HD1%)
   (( segid "BrD " and resid 74   and name HB1 ))
     3 000     2 200     2.200 peak  8402 weight  0 11000E+01 volume  0 10291E+03 ppm1     1 056 ppm2     3 563
ASSI { 8412}
   (  segid "BrD " and resid 18   and name HD1%)
   (( segid "BrD " and resid 74   and name HB2 ))
     2 900     2.100     2.100 peak  8412 weight  0 11000E+01 volume  0 13686E+03 ppm1     1 057 ppm2     2 998
ASSI { 8442}
   (  segid "BrD " and resid 18   and name HD2%)
   (  segid "BrD " and resid 14   and name HD1%)
     2.900     2 100     2 100 peak  8442 weight  0 11000E+01 volume  0 12935E+03 ppm1     0 412 ppm2     1 417
ASSI { 8452}
   (  segid "BrD " and resid 18   and name HD2%)
   (( segid "BrD " and resid 18   and name HB2 ))
     2 800     2 000     2 000 peak  8452 weight  0 11000E+01 volume  0 15454E+03 ppm1     0 415 ppm2     0 917
ASSI { 8462}
   (  segid "BrD " and resid 18   and name HD2%)
   (  segid "BrD " and resid 102  and name HD2%)
     5.500     5.500     0 000 peak  8462 weight  0.11000E+01 volume  0.22428E+01 ppm1     0 416 ppm2     1 320
ASSI { 8552}
   (( segid "BrD " and resid 22   and name HB1 ))
   (( segid "BrD " and resid 19   and name HA  ))
     2.600     1 700     1 700 peak  8552 weight  0 11000E+01 volume  0 27759E+03 ppm1     2 682 ppm2     4 295
ASSI { 8562}
   (( segid "BrD " and resid 22   and name HB2 ))
   (  segid "BrD " and resid 22   and name HD1%)
     2 500     1.600     1 600 peak  8562 weight  0 11000E+01 volume  0 30282E+03 ppm1     2 286 ppm2     1 671
ASSI { 8602}
   (( segid "BrD " and resid 22   and name HA  ))
   (( segid "BrD " and resid 25   and name HB  ))
     2.600     1 700     1 700 peak  8602 weight  0 11000E+01 volume  0 25484E+03 ppm1     4 706 ppm2     2 980
ASSI { 8652}
   (  segid "BrD " and resid 56   and name HD1%)
   (( segid "BrD " and resid 56   and name HA  ))
     2.500     1 600     1 600 peak  8652 weight  0 11000E+01 volume  0.34489E+03 ppm1     1 544 ppm2     4 638
ASSI { 8672}
   (  segid "BrD " and resid 56   and name HD2%)
   (  segid "BrD " and resid 78   and name HD2%)
     2 900     2 100     2 100 peak  8672 weight  0.11000E+01 volume  0 14779E+03 ppm1     1 253 ppm2     0 674
ASSI { 8682}
   (  segid "BrD " and resid 56   and name HD2%)
   (  segid "BrD " and resid 78   and name HD1%)
     2 300     1 300     1.300 peak  8682 weight  0 11000E+01 volume  0 48347E+03 ppm1     1 254 ppm2     0.767
ASSI { 8722}
   (( segid "BrD " and resid 73   and name HA  ))
   (  segid "BrD " and resid 76   and name HB% )
     2 700     1 800     1 800 peak  8722 weight  0 11000E+01 volume  0 22156E+03 ppm1     4 805 ppm2     2 101
ASSI { 8742}
   (  segid "BrD " and resid 73   and name HD1%)
   (( segid "BrD " and resid 73   and name HB1 ))
     2 400     1 400     1 400 peak  8742 weight  0 11000E+01 volume  0 42630E+03 ppm1     1 549 ppm2     2 594
ASSI { 8752}
   (( segid "BrD " and resid 78   and name HA  ))
   (  segid "BrD " and resid 59   and name HE% )
     3 300     2 700     2 200 peak  8752 weight  0 11000E+01 volume  0 67002E+02 ppm1     3 967 ppm2     1 876
ASSI { 8782}
   (( segid "BrD " and resid 78   and name HB1 ))
   (  segid "BrD " and resid 59   and name HE% )
     3 200     2 600     2 300 peak  8782 weight  0 11000E+01 volume  0 75592E+02 ppm1     1 307 ppm2     1 876
ASSI { 8792}
   (( segid "BrD " and resid 78   and name HB2 ))
   (  segid "BrD " and resid 59   and name HE% )
     2 900     2 100     2 100 peak  8792 weight  0 11000E+01 volume  0 13248E+03 ppm1     1 054 ppm2     1 876
ASSI { 8802}
   (( segid "BrD " and resid 78   and name HB1 ))
   (( segid "BrD " and resid 75   and name HA  ))
     3 100     2 400     2 400 peak  8802 weight  0 11000E+01 volume  0 93675E+02 ppm1     1 305 ppm2     4 520
ASSI { 8812}
   (( segid "BrD " and resid 78   and name HG  ))
   (  segid "BrD " and resid 59   and name HE% )
     3 200     2 600     2 300 peak  8812 weight  0 11000E+01 volume  0 81269E+02 ppm1     1 254 ppm2     1 878
ASSI { 8822}
   (  segid "BrD " and resid 78   and name HD1%)
   (  segid "BrD " and resid 81   and name HG1%)
     2 600     1 700     1 700 peak  8822 weight  0 11000E+01 volume  0 25375E+03 ppm1     0 761 ppm2     1 078
ASSI { 8852}
   (  segid "BrD " and resid 78   and name HD1%)
   (  segid "BrD " and resid 59   and name HE% )
     2 900     2 100     2 100 peak  8852 weight  0 11000E+01 volume  0 13937E+03 ppm1     0 761 ppm2     1 875
ASSI { 8872}
   (  segid "BrD " and resid 78   and name HD2%)
   (  segid "BrD " and resid 25   and name HG2%)
     2 600     1 700     1 700 peak  8872 weight  0 11000E+01 volume  0 25847E+03 ppm1     0 662 ppm2     1 637
ASSI { 8892}
   (  segid "BrD " and resid 78   and name HD2%)
   (  segid "BrD " and resid 81   and name HG1%)
     2.800     2 000     2 000 peak  8892 weight  0 11000E+01 volume  0 17974E+03 ppm1     0 662 ppm2     1 078
ASSI { 8912}
   (  segid "BrD " and resid 78   and name HD2%)
   (  segid "BrD " and resid 59   and name HE% )
     2.600     1.700     1 700 peak  8912 weight  0.11000E+01 volume  0 24075E+03 ppm1     0 662 ppm2     1 875
ASSI { 8922}
   (( segid "BrD " and resid 102  and name HA  ))
   (( segid "BrD " and resid 105  and name HB1 ))
     2.800     2 000     2 000 peak  8922 weight  0 11000E+01 volume  0 18319E+03 ppm1     4 263 ppm2     3 742
ASSI { 8932}
   (( segid "BrD " and resid 102  and name HA  ))
   (( segid "BrD " and resid 105  and name HB2 ))
     2 700     1 800     1 800 peak  8932 weight  0.11000E+01 volume  0 21483E+03 ppm1     4 263 ppm2     3 674
ASSI { 8952}
   (( segid "BrD " and resid 102  and name HB1 ))
   (( segid "BrD " and resid 99   and name HA  ))
     2 900     2 100     2 100 peak  8952 weight  0 11000E+01 volume  0 14144E+03 ppm1     1.993 ppm2     4.442
ASSI { 8972}
   (  segid "BrD " and resid 102  and name HD1%)
   (( segid "BrD " and resid 25   and name HA  ))
     2.700     1.800     1 800 peak  8972 weight  0 11000E+01 volume  0 20447E+03 ppm1     1 303 ppm2     4 434
ASSI { 8982}
   (  segid "BrD " and resid 102  and name HD1%)
   (( segid "BrD " and resid 105  and name HB1 ))
     3 000     2 200     2.200 peak  8982 weight  0 11000E+01 volume  0 11841E+03 ppm1     1 303 ppm2     3 760
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ASSI { 8992}
  (  segid "BrD " and resid 102  and name HD1%)
  (( segid "BrD " and resid 105  and name HB2 ))
   2 800     2 000     2 000 peak  8992 weight  0 11000E+01 volume  0 16956E+03 ppm1     1.303 ppm2     3.689
ASSI { 9002}
  (  segid "BrD " and resid 102  and name HD1%)
  (( segid "BrD " and resid 28   and name HB1 ))
   2.600     1 700     1.700 peak  9002 weight  0 11000E+01 volume  0.27744E+03 ppm1     1 303 ppm2     3 603
ASSI { 9012}
  (  segid "BrD " and resid 102  and name HD1%)
  (( segid "BrD " and resid 28   and name HB2 ))
   2 800     2.000     2 000 peak  9012 weight  0 11000E+01 volume  0 15194E+03 ppm1     1.303 ppm2     3 402
ASSI { 9062}
  (( segid "BrD " and resid 115  and name HB1 ))
  (  segid "BrD " and resid 115  and name HD1%)
   2 300     1 300     1 300 peak  9062 weight  0 11000E+01 volume  0.58334E+03 ppm1     2 190 ppm2     1 348
ASSI { 9082}
  (( segid "BrD " and resid 21   and name HA  ))
  (( segid "BrD " and resid 24   and name HB1 ))
   3 000     2 200     2 200 peak  9082 weight  0 11000E+01 volume  0 11815E+03 ppm1     4 360 ppm2     3.074
ASSI { 9092}
  (( segid "BrD " and resid 21   and name HB  ))
  (( segid "BrD " and resid 18   and name HA  ))
   2 800     2 000     2 000 peak  9092 weight  0 11000E+01 volume  0 16218E+03 ppm1     2 488 ppm2     3 884
ASSI { 9182}
  (  segid "BrD " and resid 21   and name HD1%)
  (  segid "BrD " and resid 18   and name HD2%)
   2 900     2 100     2 100 peak  9182 weight  0 11000E+01 volume  0 13133E+03 ppm1     1 203 ppm2     0 410
ASSI { 9222}
  (  segid "BrD " and resid 21   and name HD1%)
  (( segid "BrD " and resid 18   and name HA  ))
   2 900     2 100     2 100 peak  9222 weight  0 11000E+01 volume  0 13713E+03 ppm1     1 205 ppm2     3 883
ASSI { 9242}
  (( segid "BrD " and resid 50   and name HG11))
  (( segid "BrD " and resid 50   and name HG12))
   2 500     1 600     1 600 peak  9242 weight  0 11000E+01 volume  0.31586E+03 ppm1     1 397 ppm2     0 834
ASSI { 9292}
  (  segid "BrD " and resid 50   and name HG2%)
  (( segid "BrD " and resid 53   and name HB1 ))
   2 700     1 800     1 800 peak  9292 weight  0 11000E+01 volume  0 22449E+03 ppm1     1 006 ppm2     2 820
ASSI { 9302}
  (  segid "BrD " and resid 50   and name HG2%)
  (( segid "BrD " and resid 53   and name HG2 ))
   3 100     2 400     2 400 peak  9302 weight  0 11000E+01 volume  0 95431E+02 ppm1     1 006 ppm2     2 500
ASSI { 9312}
  (  segid "BrD " and resid 50   and name HG2%)
  (( segid "BrD " and resid 84   and name HB2 ))
   2 800     2 000     2 000 peak  9312 weight  0.11000E+01 volume  0 16689E+03 ppm1     1 004 ppm2     3 271
ASSI { 9322}
  (  segid "BrD " and resid 50   and name HG2%)
  (( segid "BrD " and resid 53   and name HA  ))
   2 500     1 600     1 600 peak  9322 weight  0 11000E+01 volume  0 33859E+03 ppm1     1 008 ppm2     4.690
ASSI { 9332}
  (( segid "BrD " and resid 101  and name HA  ))
  (( segid "BrD " and resid 104  and name HD1 ))
   3 000     2 200     2 200 peak  9332 weight  0 11000E+01 volume  0 11803E+03 ppm1     4 265 ppm2     2 302
ASSI { 9342}
  (( segid "BrD " and resid 101  and name HB  ))
  (( segid "BrD " and resid 98   and name HA  ))
   2 500     1 600     1.600 peak  9342 weight  0.11000E+01 volume  0 31366E+03 ppm1     2 533 ppm2     4 810
ASSI { 9372}
  (( segid "BrD " and resid 101  and name HG11))
  (( segid "BrD " and resid 101  and name HG12))
   2.300     1 300     1 300 peak  9372 weight  0 11000E+01 volume  0 48997E+03 ppm1     2 444 ppm2     1.807
ASSI { 9422}
  (  segid "BrD " and resid 101  and name HD1%)
  (( segid "BrD " and resid 98   and name HA  ))
   2 600     1 700     1 700 peak  9422 weight  0.11000E+01 volume  0 26958E+03 ppm1     1 547 ppm2     4 810
ASSI { 9432}
  (( segid "BrD " and resid 110  and name HA  ))
  (( segid "BrD " and resid 110  and name HG12))
   3 000     2 200     2 200 peak  9432 weight  0 11000E+01 volume  0 11168E+03 ppm1     4 411 ppm2     1 651
ASSI { 9442}
  (( segid "BrD " and resid 110  and name HA  ))
  (  segid "BrD " and resid 113  and name HB% )
   2.700     1 800     1 800 peak  9442 weight  0 11000E+01 volume  0 20383E+03 ppm1     4 411 ppm2     1 976
ASSI { 9712}
  (( segid "BrD " and resid 24   and name HA  ))
  (( segid "BrD " and resid 24   and name HB2 ))
   2.500     1 600     1 600 peak  9712 weight  0 11000E+01 volume  0 30771E+03 ppm1     4 784 ppm2     2 989
ASSI { 9762}
  (( segid "BrD " and resid 23   and name HA  ))
  (( segid "BrD " and resid 23   and name HB2 ))
   2 300     1 300     1 300 peak  9762 weight  0 11000E+01 volume  0 47366E+03 ppm1     4 653 ppm2     2 857
ASSI { 9772}
  (( segid "BrD " and resid 23   and name HA  ))
  (( segid "BrD " and resid 23   and name HB1 ))
   2 400     1 400     1 400 peak  9772 weight  0 11000E+01 volume  0 38829E+03 ppm1     4 653 ppm2     2 930
ASSI { 9782}
  (( segid "BrD " and resid 13   and name HB1 ))
  (( segid "BrD " and resid 13   and name HA  ))
   2 900     2.100     2 100 peak  9782 weight  0 11000E+01 volume  0 14088E+03 ppm1     2 733 ppm2     4 775
ASSI { 9802}
  (( segid "BrD " and resid 103  and name HA  ))
  (( segid "BrD " and resid 103  and name HB2 ))
   2 900     2 100     2 100 peak  9802 weight  0 11000E+01 volume  0 13225E+03 ppm1     3 769 ppm2     1 897
ASSI { 9812}
  (( segid "BrD " and resid 103  and name HA  ))
  (( segid "BrD " and resid 103  and name HB1 ))
   2 800     2 000     2 000 peak  9812 weight  0 11000E+01 volume  0.16112E+03 ppm1     3 769 ppm2     2 346
ASSI { 9822}
  (( segid "BrD " and resid 103  and name HA  ))
  (( segid "BrD " and resid 106  and name HB1 ))
   2 800     2.000     2 000 peak  9822 weight  0 11000E+01 volume  0 15761E+03 ppm1     3 769 ppm2     3 917
ASSI { 9832}
  (( segid "BrD " and resid 103  and name HA  ))
  (( segid "BrD " and resid 106  and name HB2 ))
   2 800     2 000     2.000 peak  9832 weight  0 11000E+01 volume  0.15186E+03 ppm1     3 769 ppm2     3 702
ASSI { 9862}
  (( segid "BrD " and resid 10   and name HA  ))
  (( segid "BrD " and resid 11   and name HD1 ))
   3 000     2 200     2.200 peak  9862 weight  0 11000E+01 volume  0 11074E+03 ppm1     5 479 ppm2     4 464
ASSI { 9872}
  (( segid "BrD " and resid 22   and name HB2 ))
  (( segid "BrD " and resid 19   and name HA  ))
   2 800     2 000     2 000 peak  9872 weight  0 11000E+01 volume  0 16684E+03 ppm1     2 286 ppm2     4 297
ASSI { 9912}
  (( segid "BrD " and resid 36   and name HB1 ))
  (( segid "BrD " and resid 36   and name HA  ))
   2 700     1 800     1.800 peak  9912 weight  0 11000E+01 volume  0 21618E+03 ppm1     2.685 ppm2     5 445
ASSI { 9922}
  (( segid "BrD " and resid 36   and name HB2 ))
  (( segid "BrD " and resid 36   and name HA  ))
   2 800     2 000     2 000 peak  9922 weight  0 11000E+01 volume  0 17054E+03 ppm1     2 340 ppm2     5.444
ASSI { 9932}
  (( segid "BrD " and resid 36   and name HB1 ))
  (( segid "BrD " and resid 37   and name HD1 ))
   5 500     5 500     0.000 peak  9932 weight  0 11000E+01 volume  0.21944E+00 ppm1     2 686 ppm2     4 296
ASSI { 9942}
  (( segid "BrD " and resid 36   and name HB2 ))
  (( segid "BrD " and resid 37   and name HD1 ))
   3 900     3.800     1 600 peak  9942 weight  0 11000E+01 volume  0 23373E+02 ppm1     2 341 ppm2     4 296
ASSI { 9952}
  (( segid "BrD " and resid 36   and name HG1 ))
  (( segid "BrD " and resid 37   and name HD1 ))
   2 600     1 700     1.700 peak  9952 weight  0 11000E+01 volume  0 23785E+03 ppm1     2 781 ppm2     4 289
ASSI { 9962}
  (( segid "BrD " and resid 54   and name HB1 ))
  (( segid "BrD " and resid 54   and name HA  ))
   2 900     2 100     2 100 peak  9962 weight  0 11000E+01 volume  0 14616E+03 ppm1     2 585 ppm2     5 542
ASSI { 9982}
  (( segid "BrD " and resid 54   and name HB2 ))
  (( segid "BrD " and resid 54   and name HG1 ))
   2 900     2 100     2 100 peak  9982 weight  0 11000E+01 volume  0 13342E+03 ppm1     1 947 ppm2     3 304
ASSI {10042}
  (( segid "BrD " and resid 54   and name HA  ))
  (( segid "BrD " and resid 54   and name HG1 ))
   3 400     2.900     2 100 peak 10042 weight  0.11000E+01 volume  0 51922E+02 ppm1     5 541 ppm2     3 304
ASSI {10062}
  (( segid "BrD " and resid 35   and name HA  ))
  (( segid "BrD " and resid 35   and name HB2 ))
   3 000     2 200     2 200 peak 10062 weight  0 11000E+01 volume  0 10268E+03 ppm1     4 904 ppm2     2 781
ASSI {10072}
  (( segid "BrD " and resid 35   and name HA  ))
  (( segid "BrD " and resid 35   and name HB1 ))
   3 100     2 400     2 400 peak 10072 weight  0 11000E+01 volume  0 86087E+02 ppm1     4 904 ppm2     2 831
ASSI {10112}
  (( segid "BrD " and resid 70   and name HB1 ))
  (  segid "BrD " and resid 69   and name HG2%)
   4 700     4 700     0 800 peak 10112 weight  0.11000E+01 volume  0 77364E+01 ppm1     4 756 ppm2     1 427
ASSI {10122}
  (( segid "BrD " and resid 70   and name HB2 ))
  (  segid "BrD " and resid 69   and name HG2%)
   4 800     4 800     0 700 peak 10122 weight  0 11000E+01 volume  0.67595E+01 ppm1     4 359 ppm2     1 428
ASSI {10132}
  (( segid "BrD " and resid 70   and name HB2 ))
  (  segid "BrD " and resid 69   and name HG1%)
   3 200     2 600     2 300 peak 10132 weight  0 11000E+01 volume  0 71828E+02 ppm1     4 360 ppm2     1 543
ASSI {10232}
  (( segid "BrD " and resid 7    and name HB1 ))
  (( segid "BrD " and resid 7    and name HA  ))
   2 800     2 000     2.000 peak 10232 weight  0 11000E+01 volume  0 15716E+03 ppm1     2.634 ppm2     5 143
ASSI {10242}
  (( segid "BrD " and resid 7    and name HB2 ))
  (( segid "BrD " and resid 7    and name HA  ))
   2 900     2.100     2 100 peak 10242 weight  0 11000E+01 volume  0 13922E+03 ppm1     2 501 ppm2     5.143
ASSI {10252}
  (( segid "BrD " and resid 42   and name HA  ))
  (( segid "BrD " and resid 42   and name HB1 ))
   2 400     1.400     1.400 peak 10252 weight  0.11000E+01 volume  0 37492E+03 ppm1     5 051 ppm2     2 784
ASSI {10292}
  (( segid "BrD " and resid 42   and name HB2 ))
  (( segid "BrD " and resid 42   and name HA  ))
   2 300     1 300     1 300 peak 10292 weight  0.11000E+01 volume  0 49547E+03 ppm1     2 586 ppm2     5.046
ASSI {10312}
  (( segid "BrD " and resid 87   and name HA  ))
  (( segid "BrD " and resid 87   and name HB2 ))
   2 400     1 400     1 400 peak 10312 weight  0 11000E+01 volume  0.37351E+03 ppm1     4 858 ppm2     2 581
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ASSI {10322}
   (( segid "BrD " and resid 87   and name HA  ))
   (( segid "BrD " and resid 87   and name HB1 ))
     2 500     1 600     1.600 peak 10322 weight  0.11000E+01 volume  0 30668E+03 ppm1     4 854 ppm2     2.780
ASSI {10332}
   (( segid "BrD " and resid 87   and name HB1 ))
   (( segid "BrD " and resid 84   and name HA  ))
     2 600     1.700     1 700 peak 10332 weight  0 11000E+01 volume  0.28367E+03 ppm1     2 779 ppm2     4 873
ASSI {10342}
   (( segid "BrD " and resid 87   and name HB2 ))
   (( segid "BrD " and resid 84   and name HA  ))
     2.100     1 100     1 100 peak 10342 weight  0 11000E+01 volume  0 80939E+03 ppm1     2.585 ppm2     4 873
ASSI {10352}
   (( segid "BrD " and resid 87   and name HB2 ))
   (( segid "BrD " and resid 87   and name HG1 ))
     2 300     1 300     1.300 peak 10352 weight  0 11000E+01 volume  0 47273E+03 ppm1     2 585 ppm2     3.021
ASSI {10392}
   (( segid "BrD " and resid 87   and name HG2 ))
   (  segid "BrD " and resid 50   and name HD1%)
     3 500     3 100     2 000 peak 10392 weight  0 11000E+01 volume  0 42729E+02 ppm1     2 782 ppm2     1 145
ASSI {10402}
   (( segid "BrD " and resid 48   and name HA  ))
   (( segid "BrD " and resid 48   and name HB1 ))
     2 400     1 400     1.400 peak 10402 weight  0 11000E+01 volume  0 46141E+03 ppm1     4 803 ppm2     2 729
ASSI {10422}
   (( segid "BrD " and resid 94   and name HA  ))
   (( segid "BrD " and resid 94   and name HB1 ))
     2 300     1 300     1 300 peak 10422 weight  0 11000E+01 volume  0 56402E+03 ppm1     4 831 ppm2     2 731
ASSI {10452}
   (( segid "BrD " and resid 92   and name HB2 ))
   (( segid "BrD " and resid 92   and name HA  ))
     2 300     1 300     1 300 peak 10452 weight  0 11000E+01 volume  0 48724E+03 ppm1     2 570 ppm2     4 798
ASSI {10462}
   (( segid "BrD " and resid 92   and name HB1 ))
   (( segid "BrD " and resid 92   and name HA  ))
     2 000     1 000     1 000 peak 10462 weight  0 11000E+01 volume  0 12901E+04 ppm1     2 694 ppm2     4.798
ASSI {10482}
   (( segid "BrD " and resid 112  and name HB1 ))
   (( segid "BrD " and resid 109  and name HA  ))
     2 400     1 400     1 400 peak 10482 weight  0 11000E+01 volume  0.44320E+03 ppm1     2 684 ppm2     4 638
ASSI {10492}
   (( segid "BrD " and resid 112  and name HB1 ))
   (( segid "BrD " and resid 112  and name HA  ))
     2.400     1 400     1.400 peak 10492 weight  0 11000E+01 volume  0 38447E+03 ppm1     2 684 ppm2     4.587
ASSI {10532}
   (( segid "BrD " and resid 75   and name HA  ))
   (( segid "BrD " and resid 75   and name HB1 ))
     2 500     1.600     1 600 peak 10532 weight  0 11000E+01 volume  0 36144E+03 ppm1     4 509 ppm2     2 931
ASSI {10542}
   (( segid "BrD " and resid 75   and name HA  ))
   (( segid "BrD " and resid 75   and name HB2 ))
     2 400     1 400     1 400 peak 10542 weight  0 11000E+01 volume  0 39358E+03 ppm1     4 509 ppm2     2.847
ASSI {10552}
   (( segid "BrD " and resid 75   and name HG1 ))
   (  segid "BrD " and resid 75   and name HE% )
     2 600     1 700     1 700 peak 10552 weight  0 11000E+01 volume  0 23961E+03 ppm1     3 523 ppm2     2 662
ASSI {10562}
   (( segid "BrD " and resid 75   and name HG2 ))
   (  segid "BrD " and resid 75   and name HE% )
     2.600     1 700     1.700 peak 10562 weight  0 11000E+01 volume  0.23485E+03 ppm1     3.227 ppm2     2 662
ASSI {10632}
   (( segid "BrD " and resid 66   and name HA  ))
   (( segid "BrD " and resid 66   and name HG1 ))
     2 600     1 700     1 700 peak 10632 weight  0 11000E+01 volume  0 25166E+03 ppm1     5 000 ppm2     2 181
ASSI {10642}
   (( segid "BrD " and resid 66   and name HG2 ))
   (( segid "BrD " and resid 66   and name HA  ))
     2 500     1 600     1 600 peak 10642 weight  0 11000E+01 volume  0 30460E+03 ppm1     2 141 ppm2     4 998
ASSI {10652}
   (( segid "BrD " and resid 66   and name HA  ))
   (( segid "BrD " and resid 66   and name HB1 ))
     2 300     1.300     1 300 peak 10652 weight  0 11000E+01 volume  0 48749E+03 ppm1     5 000 ppm2     2 702
ASSI {10662}
   (( segid "BrD " and resid 66   and name HA  ))
   (( segid "BrD " and resid 66   and name HB2 ))
     2.100     1 100     1 100 peak 10662 weight  0 11000E+01 volume  0 87656E+03 ppm1     5 000 ppm2     2 608
ASSI {10672}
   (( segid "BrD " and resid 80   and name HB2 ))
   (( segid "BrD " and resid 77   and name HA  ))
     2 600     1 700     1 700 peak 10672 weight  0 11000E+01 volume  0 24800E+03 ppm1     2 536 ppm2     4 951
ASSI {10682}
   (( segid "BrD " and resid 80   and name HB1 ))
   (( segid "BrD " and resid 77   and name HA  ))
     2 600     1 700     1.700 peak 10682 weight  0.11000E+01 volume  0 24031E+03 ppm1     2 583 ppm2     4.951
ASSI {10692}
   (( segid "BrD " and resid 80   and name HB2 ))
   (( segid "BrD " and resid 80   and name HA  ))
     3 000     2 200     2.200 peak 10692 weight  0 11000E+01 volume  0 11905E+03 ppm1     2 536 ppm2     4.671
ASSI {10702}
   (( segid "BrD " and resid 80   and name HB1 ))
   (( segid "BrD " and resid 80   and name HA  ))
     2 900     2 100     2.100 peak 10702 weight  0 11000E+01 volume  0 13820E+03 ppm1     2 584 ppm2     4 672
ASSI {10752}
   (( segid "BrD " and resid 80   and name HA  ))
   (( segid "BrD " and resid 80   and name HG1 ))
     2 300     1 300     1 300 peak 10752 weight  0.11000E+01 volume  0 52255E+03 ppm1     4 655 ppm2     2 339
ASSI {10762}
   (( segid "BrD " and resid 80   and name HA  ))
   (  segid "BrD " and resid 83   and name HG2%)
     3 200     2.600     2.300 peak 10762 weight  0.11000E+01 volume  0 74419E+02 ppm1     4 655 ppm2     1.901
ASSI {10792}
   (( segid "BrD " and resid 9    and name HA  ))
   (( segid "BrD " and resid 9    and name HB1 ))
     2 500     1 600     1 600 peak 10792 weight  0.11000E+01 volume  0 30562E+03 ppm1     4 953 ppm2     2 434
ASSI {10802}
   (( segid "BrD " and resid 20   and name HA  ))
   (( segid "BrD " and resid 23   and name HB1 ))
     2 800     2.000     2 000 peak 10802 weight  0 11000E+01 volume  0 14886E+03 ppm1     4 901 ppm2     2 931
ASSI {10812}
   (( segid "BrD " and resid 20   and name HA  ))
   (( segid "BrD " and resid 23   and name HB2 ))
     2 900     2 100     2.100 peak 10812 weight  0 11000E+01 volume  0 14118E+03 ppm1     4 901 ppm2     2 857
ASSI {10822}
   (( segid "BrD " and resid 27   and name HB1 ))
   (( segid "BrD " and resid 24   and name HA  ))
     2 500     1 600     1 600 peak 10822 weight  0 11000E+01 volume  0 34604E+03 ppm1     4 608 ppm2     4 788
ASSI {10932}
   (( segid "BrD " and resid 108  and name HA  ))
   (( segid "BrD " and resid 111  and name HB1 ))
     2 900     2 100     2 100 peak 10932 weight  0 11000E+01 volume  0 13575E+03 ppm1     4 801 ppm2     2 475
ASSI {10942}
   (( segid "BrD " and resid 108  and name HA  ))
   (( segid "BrD " and resid 111  and name HB2 ))
     3 000     2 200     2 200 peak 10942 weight  0 11000E+01 volume  0 11676E+03 ppm1     4 803 ppm2     2 351
ASSI {10952}
   (( segid "BrD " and resid 108  and name HA  ))
   (( segid "BrD " and resid 111  and name HD1 ))
     3 200     2 600     2.300 peak 10952 weight  0 11000E+01 volume  0 76235E+02 ppm1     4 803 ppm2     2 237
ASSI {11002}
   (( segid "BrD " and resid 44   and name HG2 ))
   (( segid "BrD " and resid 44   and name HD1 ))
     2.300     1 300     1.300 peak 11002 weight  0 11000E+01 volume  0 53477E+03 ppm1     2 645 ppm2     4 337
ASSI {11032}
   (( segid "BrD " and resid 44   and name HD1 ))
   (( segid "BrD " and resid 43   and name HA  ))
     2 300     1 300     1 300 peak 11032 weight  0 11000E+01 volume  0 59437E+03 ppm1     4 312 ppm2     5 541
ASSI {11092}
   (( segid "BrD " and resid 11   and name HA  ))
   (( segid "BrD " and resid 14   and name HB1 ))
     3 000     2.200     2.200 peak 11092 weight  0 11000E+01 volume  0 11894E+03 ppm1     4.951 ppm2     2 471
ASSI {11112}
   (( segid "BrD " and resid 11   and name HD1 ))
   (( segid "BrD " and resid 10   and name HB2 ))
     2 800     2 000     2 000 peak 11112 weight  0 11000E+01 volume  0 15710E+03 ppm1     4.457 ppm2     3 300
ASSI {11122}
   (( segid "BrD " and resid 11   and name HD1 ))
   (( segid "BrD " and resid 10   and name HB1 ))
     3 000     2 200     2.200 peak 11122 weight  0 11000E+01 volume  0 11776E+03 ppm1     4 457 ppm2     3 355
ASSI {11152}
   (( segid "BrD " and resid 37   and name HD1 ))
   (( segid "BrD " and resid 36   and name HA  ))
     3 400     2.900     2 100 peak 11152 weight  0 11000E+01 volume  0 48585E+02 ppm1     4.262 ppm2     5 446
ASSI {11182}
   (( segid "BrD " and resid 53   and name HD2 ))
   (  segid "BrD " and resid 50   and name HG2%)
     3 400     2 900     2.100 peak 11182 weight  0.11000E+01 volume  0 47917E+02 ppm1     4 015 ppm2     0 993
ASSI {11212}
   (( segid "BrD " and resid 53   and name HG1 ))
   (( segid "BrD " and resid 53   and name HD1 ))
     2 800     2 000     2 000 peak 11212 weight  0 11000E+01 volume  0 15118E+03 ppm1     2 784 ppm2     4 209
ASSI {11222}
   (( segid "BrD " and resid 53   and name HG2 ))
   (( segid "BrD " and resid 53   and name HD1 ))
     2 800     2.000     2 000 peak 11222 weight  0 11000E+01 volume  0 15165E+03 ppm1     2 490 ppm2     4 210
ASSI {11232}
   (( segid "BrD " and resid 53   and name HG2 ))
   (( segid "BrD " and resid 53   and name HD2 ))
     2 900     2 100     2 100 peak 11232 weight  0.11000E+01 volume  0 12572E+03 ppm1     2 488 ppm2     4 011
ASSI {11242}
   (( segid "BrD " and resid 53   and name HG1 ))
   (( segid "BrD " and resid 53   and name HD2 ))
     3 100     2.400     2 400 peak 11242 weight  0 11000E+01 volume  0 94017E+02 ppm1     2.784 ppm2     4 011
ASSI {11252}
   (( segid "BrD " and resid 53   and name HG1 ))
   (  segid "BrD " and resid 50   and name HG2%)
     4.300     4.300     1 200 peak 11252 weight  0 11000E+01 volume  0 13261E+02 ppm1     2.784 ppm2     0 993
ASSI {11272}
   (( segid "BrD " and resid 19   and name HB1 ))
   (  segid "BrD " and resid 63   and name HD2%)
     3 000     2 200     2 200 peak 11272 weight  0.11000E+01 volume  0 10292E+03 ppm1     2.290 ppm2     1 492
ASSI {11292}
   (( segid "BrD " and resid 19   and name HB1 ))
   (  segid "BrD " and resid 63   and name HD1%)
     3.300     2.700     2 200 peak 11292 weight  0 11000E+01 volume  0 56479E+02 ppm1     2 290 ppm2     1 655
ASSI {11302}
   (( segid "BrD " and resid 19   and name HB2 ))
   (  segid "BrD " and resid 63   and name HD1%)
     3 400     2.900     2.100 peak 11302 weight  0 11000E+01 volume  0 52899E+02 ppm1     1 988 ppm2     1 655
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ASSI {11392}
  (( segid "BrD " and resid 97   and name HA  ))
  (( segid "BrD " and resid 97   and name HG1 ))
     2 400      1 400     1 400 peak 11392 weight  0 11000E+01 volume  0 40873E+03 ppm1     4 805 ppm2     2 438
ASSI {11422}
  (( segid "BrD " and resid 97   and name HB1 ))
  (( segid "BrD " and resid 94   and name HA  ))
     2 200      1 200     1 200 peak 11422 weight  0 11000E+01 volume  0.64841E+03 ppm1     2 685 ppm2     4 830
ASSI {11442}
  (( segid "BrD " and resid 97   and name HD1 ))
  (( segid "BrD " and resid 97   and name HA  ))
     3 600      3 200     1 900 peak 11442 weight  0 11000E+01 volume  0 36224E+02 ppm1     2 420 ppm2     4 800
ASSI {11472}
  (( segid "BrD " and resid 86   and name HB1 ))
  (( segid "BrD " and resid 86   and name HA  ))
     2 400      1 400     1 400 peak 11472 weight  0.11000E+01 volume  0 38167E+03 ppm1     2 340 ppm2     4 807
ASSI {11482}
  (( segid "BrD " and resid 86   and name HB1 ))
  (( segid "BrD " and resid 86   and name HG2 ))
     2 900      2 100     2.100 peak 11482 weight  0 11000E+01 volume  0 12261E+03 ppm1     2 340 ppm2     0 766
ASSI {11612}
  (( segid "BrD " and resid 64   and name HB1 ))
  (( segid "BrD " and resid 61   and name HA  ))
     2 300      1 300     1 300 peak 11612 weight  0 11000E+01 volume  0 48201E+03 ppm1     2 636 ppm2     4 667
ASSI {11622}
  (( segid "BrD " and resid 64   and name HG1 ))
  (( segid "BrD " and resid 61   and name HA  ))
     2 600      1 700     1 700 peak 11622 weight  0 11000E+01 volume  0 27263E+03 ppm1     2 190 ppm2     4 667
ASSI {11692}
  (( segid "BrD " and resid 6    and name HA  ))
  (( segid "BrD " and resid 6    and name HB2 ))
     2 400      1 400     1 400 peak 11692 weight  0 11000E+01 volume  0.40526E+03 ppm1     4 972 ppm2     2 291
ASSI {11702}
  (( segid "BrD " and resid 72   and name HD1 ))
  (( segid "BrD " and resid 72   and name HA  ))
     2 600      1 700     1.700 peak 11702 weight  0 11000E+01 volume  0 26243E+03 ppm1     2 291 ppm2     4 646
ASSI {11712}
  (( segid "BrD " and resid 62   and name HD1 ))
  (( segid "BrD " and resid 62   and name HG1 ))
     2 700      1 800     1 800 peak 11712 weight  0 11000E+01 volume  0 19040E+03 ppm1     3 177 ppm2     2 323
ASSI {11732}
  (( segid "BrD " and resid 62   and name HD2 ))
  (( segid "BrD " and resid 62   and name HG2 ))
     3 200      2 600     2 300 peak 11732 weight  0 11000E+01 volume  0 69523E+02 ppm1     2 629 ppm2     1 480
ASSI {11742}
  (( segid "BrD " and resid 62   and name HD1 ))
  (( segid "BrD " and resid 59   and name HA  ))
     3 100      2 400     2 400 peak 11742 weight  0 11000E+01 volume  0 81736E+02 ppm1     3 177 ppm2     4 911
ASSI {11782}
  (( segid "BrD " and resid 91   and name HG1 ))
  (( segid "BrD " and resid 91   and name HD2 ))
     3 000      2 200     2.200 peak 11782 weight  0 11000E+01 volume  0 11953E+03 ppm1     2 779 ppm2     4 406
ASSI {11802}
  (( segid "BrD " and resid 91   and name HA  ))
  (( segid "BrD " and resid 91   and name HB1 ))
     2.700      1 800     1 800 peak 11802 weight  0 11000E+01 volume  0.18443E+03 ppm1     5 347 ppm2     2 978
ASSI {11812}
  (( segid "BrD " and resid 91   and name HA  ))
  (( segid "BrD " and resid 91   and name HG1 ))
     3 700      3 400     1 800 peak 11812 weight  0 11000E+01 volume  0 32384E+02 ppm1     5.347 ppm2     2 788
ASSI {11852}
  (( segid "BrD " and resid 91   and name HD1 ))
  (( segid "BrD " and resid 89   and name HA  ))
     2 700      1 800     1 800 peak 11852 weight  0 11000E+01 volume  0 19122E+03 ppm1     4 559 ppm2     5 642
ASSI {11882}
  (( segid "BrD " and resid 91   and name HD2 ))
  (( segid "BrD " and resid 89   and name HB1 ))
     2 800      2 000     2 000 peak 11882 weight  0 11000E+01 volume  0 16587E+03 ppm1     4 410 ppm2     3 668
ASSI {11912}
  (( segid "BrD " and resid 91   and name HB2 ))
  (( segid "BrD " and resid 91   and name HD1 ))
     3 700      3 400     1.800 peak 11912 weight  0 11000E+01 volume  0 31825E+02 ppm1     2 730 ppm2     4 559
ASSI {11922}
  (( segid "BrD " and resid 91   and name HB1 ))
  (( segid "BrD " and resid 91   and name HD1 ))
     3 400      2 900     2 100 peak 11922 weight  0.11000E+01 volume  0 50256E+02 ppm1     2 978 ppm2     4 559
ASSI {11942}
  (( segid "BrD " and resid 91   and name HB2 ))
  (( segid "BrD " and resid 91   and name HA  ))
     2 800      2 000     2 000 peak 11942 weight  0 11000E+01 volume  0 17033E+03 ppm1     2 725 ppm2     5 378
ASSI {11952}
  (( segid "BrD " and resid 33   and name HA  ))
  (( segid "BrD " and resid 33   and name HG2 ))
     3 000      2 200     2 200 peak 11952 weight  0 11000E+01 volume  0 10731E+03 ppm1     4 361 ppm2    -0 319
ASSI {11962}
  (( segid "BrD " and resid 33   and name HA  ))
  (( segid "BrD " and resid 33   and name HB2 ))
     2 700      1 800     1 800 peak 11962 weight  0 11000E+01 volume  0 20069E+03 ppm1     4 361 ppm2    -0 166
ASSI {11972}
  (( segid "BrD " and resid 33   and name HA  ))
  (( segid "BrD " and resid 33   and name HB1 ))
     2 700      1 800     1.800 peak 11972 weight  0 11000E+01 volume  0 18669E+03 ppm1     4 360 ppm2     1 083
ASSI {12032}
  (( segid "BrD " and resid 33   and name HG1 ))
  (( segid "BrD " and resid 33   and name HB2 ))
     2 900      2 100     2.100 peak 12032 weight  0.11000E+01 volume  0 13883E+03 ppm1     0.858 ppm2    -0 165
ASSI {12042}
  (( segid "BrD " and resid 33   and name HG2 ))
  (( segid "BrD " and resid 33   and name HB2 ))
     2 900      2 100     2 100 peak 12042 weight  0 11000E+01 volume  0.12386E+03 ppm1    -0 324 ppm2    -0 169
ASSI {12062}
  (( segid "BrD " and resid 33   and name HD1 ))
  (( segid "BrD " and resid 33   and name HG1 ))
     3 000      2 200     2 200 peak 12062 weight  0 11000E+01 volume  0 11534E+03 ppm1     2 780 ppm2     0 864
ASSI {12072}
  (( segid "BrD " and resid 33   and name HD2 ))
  (( segid "BrD " and resid 33   and name HG1 ))
     3 100      2 400     2 400 peak 12072 weight  0 11000E+01 volume  0 97683E+02 ppm1     2 189 ppm2     0 864
ASSI {12082}
  (( segid "BrD " and resid 33   and name HD1 ))
  (( segid "BrD " and resid 33   and name HG2 ))
     2 900      2 100     2 100 peak 12082 weight  0 11000E+01 volume  0 13243E+03 ppm1     2 780 ppm2    -0 319
ASSI {12092}
  (( segid "BrD " and resid 33   and name HD2 ))
  (( segid "BrD " and resid 33   and name HG2 ))
     2 900      2 100     2 100 peak 12092 weight  0 11000E+01 volume  0 13995E+03 ppm1     2 189 ppm2    -0 319
ASSI {12102}
  (( segid "BrD " and resid 33   and name HB1 ))
  (( segid "BrD " and resid 33   and name HG2 ))
     2 900      2 100     2 100 peak 12102 weight  0 11000E+01 volume  0 14146E+03 ppm1     1 051 ppm2    -0.316
ASSI {12132}
  (( segid "BrD " and resid 33   and name HB1 ))
  (( segid "BrD " and resid 33   and name HG1 ))
     3 100      2 400     2 400 peak 12132 weight  0 11000E+01 volume  0 94205E+02 ppm1     1 055 ppm2     0 859
ASSI {12182}
  (( segid "BrD " and resid 35   and name HA  ))
  (( segid "BrD " and resid 36   and name HB1 ))
     4 100      4 100     1 400 peak 12182 weight  0 11000E+01 volume  0 16299E+02 ppm1     4 904 ppm2     2 685
ASSI {12222}
  (( segid "BrD " and resid 59   and name HG2 ))
  (  segid "BrD " and resid 59   and name HE% )
     2 300      1 300     1 300 peak 12222 weight  0 11000E+01 volume  0 52760E+03 ppm1     3 137 ppm2     1 875
ASSI {12242}
  (( segid "BrD " and resid 59   and name HB2 ))
  (  segid "BrD " and resid 59   and name HE% )
     2 700      1 800     1 800 peak 12242 weight  0 11000E+01 volume  0 19334E+03 ppm1     2 487 ppm2     1 876
ASSI {12252}
  (( segid "BrD " and resid 59   and name HA  ))
  (( segid "BrD " and resid 59   and name HB2 ))
     3 300      2 700     2 200 peak 12252 weight  0 11000E+01 volume  0 59031E+02 ppm1     4.903 ppm2     2 487
ASSI {12262}
  (( segid "BrD " and resid 59   and name HA  ))
  (( segid "BrD " and resid 62   and name HB1 ))
     3 100      2 400     2.400 peak 12262 weight  0 11000E+01 volume  0 90578E+02 ppm1     4 903 ppm2     2 657
ASSI {12272}
  (( segid "BrD " and resid 59   and name HA  ))
  (( segid "BrD " and resid 62   and name HB2 ))
     2 900      2.100     2 100 peak 12272 weight  0.11000E+01 volume  0 13057E+03 ppm1     4 903 ppm2     1.670
ASSI {12312}
  (( segid "BrD " and resid 61   and name HB1 ))
  (( segid "BrD " and resid 61   and name HA  ))
     2 500      1 600     1 600 peak 12312 weight  0 11000E+01 volume  0 30078E+03 ppm1     2 826 ppm2     4 673
ASSI {12322}
  (( segid "BrD " and resid 61   and name HB1 ))
  (( segid "BrD " and resid 58   and name HA  ))
     3.000      2 200     2 200 peak 12322 weight  0 11000E+01 volume  0 10826E+03 ppm1     2 826 ppm2     4.451
ASSI {12332}
  (( segid "BrD " and resid 61   and name HB2 ))
  (( segid "BrD " and resid 58   and name HA  ))
     2 400      1.400     1 400 peak 12332 weight  0 11000E+01 volume  0 42931E+03 ppm1     2.679 ppm2     4 453
ASSI {12342}
  (( segid "BrD " and resid 61   and name HB2 ))
  (( segid "BrD " and resid 61   and name HA  ))
     2 100      1 100     1 100 peak 12342 weight  0 11000E+01 volume  0.81117E+03 ppm1     2 679 ppm2     4 673
ASSI {12392}
  (  segid "BrD " and resid 102  and name HD2%)
  (( segid "BrD " and resid 102  and name HG  ))
     2.000      1 000     1 000 peak 12392 weight  0.11000E+01 volume  0 13882E+04 ppm1     1 304 ppm2     2.159
ASSI {12402}
  (  segid "BrD " and resid 102  and name HD2%)
  (( segid "BrD " and resid 102  and name HB1 ))
     2 400      1 400     1.400 peak 12402 weight  0 11000E+01 volume  0 42022E+03 ppm1     1 304 ppm2     2 020
ASSI {12422}
  (  segid "BrD " and resid 102  and name HD2%)
  (  segid "BrD " and resid 31   and name HB% )
     3 500      3 100     2 000 peak 12422 weight  0.11000E+01 volume  0 40319E+02 ppm1     1 305 ppm2     2.315
ASSI {12432}
  (  segid "BrD " and resid 14   and name HD1%)
  (( segid "BrD " and resid 14   and name HG  ))
     2 400      1 400     1 400 peak 12432 weight  0.11000E+01 volume  0 38368E+03 ppm1     1.402 ppm2     2.062
ASSI {12442}
  (  segid "BrD " and resid 14   and name HD1%)
  (( segid "BrD " and resid 14   and name HB2 ))
     2 300      1 300     1 300 peak 12442 weight  0 11000E+01 volume  0 51224E+03 ppm1     1.402 ppm2     2.155
ASSI {12452}
  (  segid "BrD " and resid 14   and name HD1%)
  (( segid "BrD " and resid 14   and name HB1 ))
     2 300      1 300     1 300 peak 12452 weight  0 11000E+01 volume  0 51311E+03 ppm1     1 402 ppm2     2.468
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ASSI {12462}
   ( segid "BrD " and resid 14    and name HD1%)
  (( segid "BrD " and resid 14    and name HA  ))
     2 600      1 700      1 700 peak 12462 weight  0 11000E+01 volume  0 23971E+03 ppm1    1 401 ppm2    4 655
ASSI {12472}
   ( segid "BrD " and resid 14    and name HD1%)
   ( segid "BrD " and resid 18    and name HD1%)
     2 500      1.600      1 600 peak 12472 weight  0 11000E+01 volume  0 29352E+03 ppm1    1 402 ppm2    1 084
ASSI {12602}
   ( segid "BrD " and resid 59    and name HE% )
  (( segid "BrD " and resid 59    and name HB1 ))
     2 700      1 800      1 800 peak 12602 weight  0 11000E+01 volume  0 21211E+03 ppm1    1 847 ppm2    2 707
ASSI {12622}
   ( segid "BrD " and resid 59    and name HE% )
  (( segid "BrD " and resid 59    and name HG1 ))
     3 100      2 400      2 400 peak 12622 weight  0 11000E+01 volume  0 88634E+02 ppm1    1 848 ppm2    3 230
ASSI {12662}
   ( segid "BrD " and resid 54    and name HE% )
  (( segid "BrD " and resid 54    and name HB2 ))
     2 700      1.800      1 800 peak 12662 weight  0 11000E+01 volume  0 21213E+03 ppm1    2.535 ppm2    1 964
ASSI {12682}
   ( segid "BrD " and resid 54    and name HE% )
  (( segid "BrD " and resid 54    and name HG1 ))
     2 500      1 600      1 600 peak 12682 weight  0.11000E+01 volume  0 35414E+03 ppm1    2.535 ppm2    3 307
ASSI {12772}
   ( segid "BrD " and resid 50    and name HG2%)
  (( segid "BrD " and resid 84    and name HB1 ))
     2 900      2 100      2 100 peak 12772 weight  0 11000E+01 volume  0 14057E+03 ppm1    1 004 ppm2    3 605
ASSI {12802}
  (( segid "BrD " and resid 78    and name HB2 ))
  (( segid "BrD " and resid 75    and name HA  ))
     3.300      2 700      2 200 peak 12802 weight  0 11000E+01 volume  0 66311E+02 ppm1    1 054 ppm2    4 517
ASSI {12902}
   ( segid "BrD " and resid 38    and name HG1%)
   ( segid "BrD " and resid 43    and name HB% )
     2 800      2 000      2 000 peak 12902 weight  0 11000E+01 volume  0 17186E+03 ppm1    1 059 ppm2    1 715
ASSI {12912}
  (( segid "BrD " and resid 25    and name HA  ))
  (( segid "BrD " and resid 28    and name HB2 ))
     3 400      2 900      2 100 peak 12912 weight  0 11000E+01 volume  0 50976E+02 ppm1    4 412 ppm2    3 406
ASSI {12922}
  (( segid "BrD " and resid 25    and name HA  ))
  (( segid "BrD " and resid 28    and name HB1 ))
     3 400      2 900      2 100 peak 12922 weight  0 11000E+01 volume  0 50633E+02 ppm1    4 412 ppm2    3 607
ASSI {12932}
  (( segid "BrD " and resid 25    and name HB  ))
  (( segid "BrD " and resid 25    and name HA  ))
     2 600      1 700      1.700 peak 12932 weight  0 11000E+01 volume  0 25503E+03 ppm1    2 979 ppm2    4 436
ASSI {12942}
  (( segid "BrD " and resid 99    and name HA  ))
   ( segid "BrD " and resid 102   and name HD1%)
     3 500      3 100      2 000 peak 12942 weight  0 11000E+01 volume  0 42963E+02 ppm1    4 458 ppm2    1 321
ASSI {12952}
   ( segid "BrD " and resid 17    and name HG2%)
   ( segid "BrD " and resid 18    and name HD1%)
     3.100      2 400      2 400 peak 12952 weight  0 11000E+01 volume  0 90746E+02 ppm1    1 745 ppm2    1 083
ASSI {12982}
  (( segid "BrD " and resid 98    and name HB1 ))
  (( segid "BrD " and resid 95    and name HA  ))
     3 200      2 600      2 300 peak 12982 weight  0 11000E+01 volume  0 76248E+02 ppm1    4 013 ppm2    4 445
ASSI {13062}
   ( segid "BrD " and resid 56    and name HD1%)
  (( segid "BrD " and resid 34    and name HB2 ))
     2 900      2 100      2 100 peak 13062 weight  0 11000E+01 volume  0 13096E+03 ppm1    1 546 ppm2    3 143
ASSI {13152}
  (( segid "BrD " and resid 81    and name HA  ))
  (( segid "BrD " and resid 84    and name HB2 ))
     3 300      2 700      2 200 peak 13152 weight  0 11000E+01 volume  0 59764E+02 ppm1    3 718 ppm2    3 278
ASSI {13162}
  (( segid "BrD " and resid 85    and name HA  ))
  (( segid "BrD " and resid 88    and name HB1 ))
     3 400      2 900      2 100 peak 13162 weight  0 11000E+01 volume  0 52965E+02 ppm1    5 003 ppm2    3 532
ASSI {13172}
  (( segid "BrD " and resid 86    and name HB1 ))
  (( segid "BrD " and resid 83    and name HA  ))
     3 700      3 400      1 800 peak 13172 weight  0 11000E+01 volume  0 32755E+02 ppm1    2 340 ppm2    4 462
ASSI {13182}
   ( segid "BrD " and resid 54    and name HE% )
  (( segid "BrD " and resid 54    and name HA  ))
     2 300      1 300      1 300 peak 13182 weight  0 11000E+01 volume  0 48303E+03 ppm1    2 535 ppm2    5 543
ASSI {13212}
  (( segid "BrD " and resid 47    and name HA  ))
  (( segid "BrD " and resid 50    and name HB  ))
     3 600      3 200      1 900 peak 13212 weight  0.11000E+01 volume  0.37838E+02 ppm1    4.704 ppm2    1 823
ASSI {13222}
   ( segid "BrD " and resid 81    and name HG2%)
  (( segid "BrD " and resid 34    and name HB2 ))
     2 800      2 000      2 000 peak 13222 weight  0 11000E+01 volume  0 16892E+03 ppm1    0 756 ppm2    3.149
ASSI {13252}
  (( segid "BrD " and resid 34    and name HB2 ))
  (( segid "BrD " and resid 56    and name HG  ))
     3 100      2 400      2 400 peak 13252 weight  0 11000E+01 volume  0.87944E+02 ppm1    3 127 ppm2    2 323
ASSI {13262}
  (( segid "BrD " and resid 34    and name HB1 ))
  (( segid "BrD " and resid 56    and name HG  ))
     3.200      2.600      2.300 peak 13262 weight  0 11000E+01 volume  0 75137E+02 ppm1    4 108 ppm2    2 322
ASSI {13362}
   ( segid "BrD " and resid 18    and name HD1%)
  (( segid "BrD " and resid 18    and name HB1 ))
     2.300      1 300      1 300 peak 13362 weight  0.11000E+01 volume  0 50793E+03 ppm1    1.058 ppm2    2 128
ASSI {13372}
  (( segid "BrD " and resid 14    and name HB1 ))
   ( segid "BrD " and resid 18    and name HD1%)
     4 000      4 000      1.500 peak 13372 weight  0 11000E+01 volume  0 18693E+02 ppm1    2 441 ppm2    1 084
ASSI {13382}
   ( segid "BrD " and resid 25    and name HG1%)
  (( segid "BrD " and resid 22    and name HA  ))
     2.600      1.700      1 700 peak 13382 weight  0 11000E+01 volume  0 28896E+03 ppm1    1.795 ppm2    4 720
ASSI {13402}
  (( segid "BrD " and resid 102   and name HB2 ))
  (( segid "BrD " and resid 99    and name HA  ))
     2.600      1 700      1 700 peak 13402 weight  0 11000E+01 volume  0 26245E+03 ppm1    1 842 ppm2    4 441
ASSI {13422}
  (( segid "BrD " and resid 21    and name HB  ))
   ( segid "BrD " and resid 18    and name HD2%)
     3 700      3 400      1 800 peak 13422 weight  0 11000E+01 volume  0 29780E+02 ppm1    2.487 ppm2    0 409
ASSI {13432}
  (( segid "BrD " and resid 57    and name HA  ))
  (( segid "BrD " and resid 60    and name HB2 ))
     2 700      1.800      1 800 peak 13432 weight  0 11000E+01 volume  0 19090E+03 ppm1    4 805 ppm2    4 625
ASSI {13442}
  (( segid "BrD " and resid 57    and name HA  ))
  (( segid "BrD " and resid 60    and name HB1 ))
     2 900      2.100      2 100 peak 13442 weight  0 11000E+01 volume  0 14250E+03 ppm1    4.805 ppm2    5 000
ASSI {13482}
   ( segid "BrD " and resid 58    and name HG2%)
  (( segid "BrD " and resid 62    and name HD2 ))
     2 800      2 000      2 000 peak 13482 weight  0 11000E+01 volume  0 17578E+03 ppm1    1 651 ppm2    2 644
ASSI {13492}
  (( segid "BrD " and resid 61    and name HB1 ))
   ( segid "BrD " and resid 58    and name HG2%)
     3 600      3 200      1 900 peak 13492 weight  0 11000E+01 volume  0 34592E+02 ppm1    2 826 ppm2    1 662
ASSI {13512}
   ( segid "BrD " and resid 59    and name HE% )
  (( segid "BrD " and resid 59    and name HA  ))
     3 100      2.400      2 400 peak 13512 weight  0 11000E+01 volume  0 83827E+02 ppm1    1.848 ppm2    4 913
ASSI {13522}
   ( segid "BrD " and resid 59    and name HE% )
   ( segid "BrD " and resid 56    and name HD2%)
     3 400      2 900      2 100 peak 13522 weight  0 11000E+01 volume  0 55813E+02 ppm1    1 848 ppm2    1.271
ASSI {13542}
  (( segid "BrD " and resid 21    and name HA  ))
  (( segid "BrD " and resid 24    and name HB2 ))
     3 200      2 600      2 300 peak 13542 weight  0 11000E+01 volume  0 69544E+02 ppm1    4 360 ppm2    2 989
ASSI {13552}
  (( segid "BrD " and resid 74    and name HB2 ))
  (( segid "BrD " and resid 71    and name HA  ))
     3 300      2 700      2 200 peak 13552 weight  0.11000E+01 volume  0 56669E+02 ppm1    2 974 ppm2    4 624
ASSI {13652}
   ( segid "BrD " and resid 58    and name HG2%)
  (( segid "BrD " and resid 62    and name HD1 ))
     2 800      2.000      2 000 peak 13652 weight  0 11000E+01 volume  0 18084E+03 ppm1    1 649 ppm2    3 182
ASSI {13662}
  (( segid "BrD " and resid 32    and name HA  ))
   ( segid "BrD " and resid 31    and name HB% )
     3 700      3 400      1 800 peak 13662 weight  0 11000E+01 volume  0 29321E+02 ppm1    4 952 ppm2    2 312
ASSI {13702}
  (( segid "BrD " and resid 42    and name HB1 ))
   ( segid "BrD " and resid 43    and name HB% )
     3 800      3 600      1 700 peak 13702 weight  0 11000E+01 volume  0 26752E+02 ppm1    2.785 ppm2    1 712
ASSI {13722}
  (( segid "BrD " and resid 59    and name HA  ))
  (( segid "BrD " and resid 62    and name HD2 ))
     2 600      1 700      1 700 peak 13722 weight  0.11000E+01 volume  0 25810E+03 ppm1    4 903 ppm2    2 634
ASSI {13742}
  (( segid "BrD " and resid 63    and name HG  ))
  (( segid "BrD " and resid 63    and name HB1 ))
     2 300      1 300      1 300 peak 13742 weight  0 11000E+01 volume  0 59564E+03 ppm1    2 437 ppm2    2 905
ASSI {13902}
  (( segid "BrD " and resid 70    and name HB1 ))
   ( segid "BrD " and resid 69    and name HG1%)
     3 700      3 400      1 800 peak 13902 weight  0 11000E+01 volume  0 30896E+02 ppm1    4.756 ppm2    1 544
ASSI {13912}
   ( segid "BrD " and resid 101   and name HG2%)
  (( segid "BrD " and resid 98    and name HA  ))
     2 800      2 000      2 000 peak 13912 weight  0 11000E+01 volume  0 17496E+03 ppm1    1 596 ppm2    4 810
ASSI {13932}
  (( segid "BrD " and resid 101   and name HG12))
  (( segid "BrD " and resid 98    and name HA  ))
     3 400      2 900      2 100 peak 13932 weight  0.11000E+01 volume  0 55145E+02 ppm1    1 797 ppm2    4 808
ASSI {13942}
  (( segid "BrD " and resid 98    and name HA  ))
  (( segid "BrD " and resid 101   and name HG11))
     3.300      2 700      2 200 peak 13942 weight  0 11000E+01 volume  0 65568E+02 ppm1    4 804 ppm2    2 469
ASSI {14002}
  (( segid "BrD " and resid 53    and name HB1 ))
  (( segid "BrD " and resid 53    and name HD1 ))
     2 800      2 000      2 000 peak 14002 weight  0 11000E+01 volume  0 16043E+03 ppm1    2.781 ppm2    4.208
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ASSI {14012}
  (( segid "BrD " and resid 53   and name HB1 ))
  (( segid "BrD " and resid 53   and name HD2 ))
    3.000    2 200    2 200 peak 14012 weight  0 11000E+01 volume  0 10929E+03 ppm1     2 781 ppm2     4 010
ASSI {14072}
  (( segid "BrD " and resid 79   and name HA  ))
  (( segid "BrD " and resid 82   and name HB2 ))
    3 000    2 200    2 200 peak 14072 weight  0 11000E+01 volume  0.11123E+03 ppm1     4 409 ppm2     3.606
ASSI {14082}
  (( segid "BrD " and resid 79   and name HA  ))
  (( segid "BrD " and resid 82   and name HB1 ))
    3.300    2 700    2 200 peak 14082 weight  0 11000E+01 volume  0 67314E+02 ppm1     4 409 ppm2     3 697
ASSI {14092}
  (( segid "BrD " and resid 79   and name HB2 ))
  (( segid "BrD " and resid 76   and name HA  ))
    2 400    1 400    1 400 peak 14092 weight  0 11000E+01 volume  0.38186E+03 ppm1     2 680 ppm2     4 683
ASSI {14182}
  (( segid "BrD " and resid 94   and name HA  ))
  (( segid "BrD " and resid 97   and name HD1 ))
    3.200    2 600    2 300 peak 14182 weight  0.11000E+01 volume  0 68636E+02 ppm1     4 830 ppm2     2 434
ASSI {14252}
  (( segid "BrD " and resid 113  and name HA  ))
  (  segid "BrD " and resid 17   and name HG2%)
    3.600    3 200    1 900 peak 14252 weight  0 11000E+01 volume  0 37471E+02 ppm1     4 901 ppm2     1.750
ASSI {14552}
  (( segid "BrD " and resid 11   and name HB2 ))
  (( segid "BrD " and resid 11   and name HD1 ))
    2 700    1.800    1.800 peak 14552 weight  0 11000E+01 volume  0 21551E+03 ppm1     2 580 ppm2     4 460
ASSI {14572}
  (( segid "BrD " and resid 14   and name HB2 ))
  (( segid "BrD " and resid 11   and name HA  ))
    3 300    2 700    2 200 peak 14572 weight  0 11000E+01 volume  0.58722E+02 ppm1     2 145 ppm2     4 942
ASSI {14592}
  (  segid "BrD " and resid 102  and name HD2%)
  (( segid "BrD " and resid 31   and name HA  ))
    3 400    2 900    2.100 peak 14592 weight  0 11000E+01 volume  0 51768E+02 ppm1     1 303 ppm2     4 984
ASSI {14612}
  (  segid "BrD " and resid 102  and name HD2%)
  (  segid "BrD " and resid 25   and name HG2%)
    2.300    1 300    1 300 peak 14612 weight  0 11000E+01 volume  0.50747E+03 ppm1     1 305 ppm2     1 633
ASSI {14622}
  (  segid "BrD " and resid 102  and name HD2%)
  (( segid "BrD " and resid 25   and name HA  ))
    2 700    1.800    1 800 peak 14622 weight  0 11000E+01 volume  0 22785E+03 ppm1     1 303 ppm2     4 425
ASSI {14662}
  (( segid "BrD " and resid 18   and name HB2 ))
  (( segid "BrD " and resid 18   and name HG  ))
    3 100    2 400    2 400 peak 14662 weight  0 11000E+01 volume  0 98423E+02 ppm1     0 911 ppm2     2 274
ASSI {14772}
  (( segid "BrD " and resid 36   and name HA  ))
  (( segid "BrD " and resid 37   and name HG2 ))
    5 500    5 500    0 000 peak 14772 weight  0 11000E+01 volume  0.48374E+00 ppm1     5 447 ppm2     2 587
ASSI {14812}
  (( segid "BrD " and resid 42   and name HB2 ))
  (  segid "BrD " and resid 43   and name HB% )
    3.200    2 600    2.300 peak 14812 weight  0.11000E+01 volume  0 74053E+02 ppm1     2 586 ppm2     1 710
ASSI {14822}
  (( segid "BrD " and resid 35   and name HA  ))
  (( segid "BrD " and resid 36   and name HB2 ))
    3 800    3 600    1.700 peak 14822 weight  0 11000E+01 volume  0 27804E+02 ppm1     4 904 ppm2     2 340
ASSI {14942}
  (( segid "BrD " and resid 46   and name HA  ))
  (  segid "BrD " and resid 88   and name HE% )
    2 700    1 800    1 800 peak 14942 weight  0.11000E+01 volume  0 19889E+03 ppm1     4 163 ppm2     7.421
ASSI {14962}
  (( segid "BrD " and resid 46   and name HA  ))
  (  segid "BrD " and resid 46   and name HE% )
    3 600    3.200    1.900 peak 14962 weight  0 11000E+01 volume  0.36218E+02 ppm1     4 164 ppm2     6 689
ASSI {14992}
  (( segid "BrD " and resid 46   and name HB2 ))
  (  segid "BrD " and resid 46   and name HE% )
    3 700    3 400    1 800 peak 14992 weight  0 11000E+01 volume  0 28675E+02 ppm1     3 078 ppm2     6 689
ASSI {15062}
  (( segid "BrD " and resid 28   and name HB2 ))
  (( segid "BrD " and resid 28   and name HD2 ))
    3 100    2 400    2 400 peak 15062 weight  0 11000E+01 volume  0 98530E+02 ppm1     3 372 ppm2     5.575
ASSI {15072}
  (( segid "BrD " and resid 28   and name HB1 ))
  (( segid "BrD " and resid 28   and name HD2 ))
    3 200    2 600    2 300 peak 15072 weight  0 11000E+01 volume  0 74212E+02 ppm1     3.570 ppm2     5.575
ASSI {15122}
  (( segid "BrD " and resid 67   and name HB1 ))
  (  segid "BrD " and resid 67   and name HE% )
    4.100    4 100    1 400 peak 15122 weight  0 11000E+01 volume  0 17734E+02 ppm1     2 639 ppm2     7.315
ASSI {15292}
  (( segid "BrD " and resid 47   and name HA  ))
  (  segid "BrD " and resid 46   and name HD% )
    4 100    4 100    1 400 peak 15292 weight  0 11000E+01 volume  0 16402E+02 ppm1     4.705 ppm2     5 762
ASSI {15322}
  (( segid "BrD " and resid 47   and name HB2 ))
  (  segid "BrD " and resid 47   and name HE% )
    3.400    2 900    2 100 peak 15322 weight  0 11000E+01 volume  0 56146E+02 ppm1     3 375 ppm2     7 271
ASSI {15332}
  (( segid "BrD " and resid 47   and name HB1 ))
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  (  segid "BrD " and resid 47   and name HE% )
    3 200    2 600    2 300 peak 15332 weight  0 11000E+01 volume  0 74345E+02 ppm1     3 816 ppm2     7 271
ASSI {15352}
  (( segid "BrD " and resid 32   and name HB2 ))
  (( segid "BrD " and resid 32   and name HE3 ))
    2 600    1 700    1 700 peak 15352 weight  0.11000E+01 volume  0 27498E+03 ppm1     3 962 ppm2     7 952
ASSI {15432}
  (( segid "BrD " and resid 74   and name HB1 ))
  (  segid "BrD " and resid 74   and name HD% )
    2.900    2 100    2.100 peak 15432 weight  0.11000E+01 volume  0 14689E+03 ppm1     3 576 ppm2     6 998
ASSI {15482}
  (( segid "BrD " and resid 74   and name HB2 ))
  (  segid "BrD " and resid 74   and name HE% )
    3.600    3.200    1 900 peak 15482 weight  0 11000E+01 volume  0 37941E+02 ppm1     2 985 ppm2     7 533
ASSI {15492}
  (( segid "BrD " and resid 74   and name HB1 ))
  (  segid "BrD " and resid 74   and name HE% )
    2 800    2 000    2 000 peak 15492 weight  0 11000E+01 volume  0 16094E+03 ppm1     3 571 ppm2     7 535
ASSI {15602}
  (( segid "BrD " and resid 82   and name HB2 ))
  (  segid "BrD " and resid 82   and name HE% )
    3 000    2 200    2.200 peak 15602 weight  0 11000E+01 volume  0 11655E+03 ppm1     3 573 ppm2     7 069
ASSI {15612}
  (( segid "BrD " and resid 82   and name HB1 ))
  (  segid "BrD " and resid 82   and name HE% )
    2 800    2 000    2 000 peak 15612 weight  0.11000E+01 volume  0 15106E+03 ppm1     3 672 ppm2     7 069
ASSI {15732}
  (( segid "BrD " and resid 82   and name HA  ))
  (  segid "BrD " and resid 82   and name HE% )
    3 200    2 600    2 300 peak 15732 weight  0 11000E+01 volume  0 68425E+02 ppm1     4 755 ppm2     7 063
ASSI {15742}
  (( segid "BrD " and resid 82   and name HA  ))
  (  segid "BrD " and resid 82   and name HD% )
    2 100    1 100    1.100 peak 15742 weight  0 11000E+01 volume  0 82972E+03 ppm1     4 755 ppm2     7 259
ASSI {15792}
  (( segid "BrD " and resid 15   and name HA  ))
  (  segid "BrD " and resid 18   and name HD2%)
    4.600    4 600    0 900 peak 15792 weight  0 11000E+01 volume  0 83712E+01 ppm1     4 607 ppm2     0 408
ASSI {16522}
  (( segid "BrD " and resid 107  and name HA  ))
  (  segid "BrD " and resid 107  and name HE% )
    2.700    1 800    1 800 peak 16522 weight  0.11000E+01 volume  0 21131E+03 ppm1     4 410 ppm2     7 901
ASSI {16532}
  (( segid "BrD " and resid 96   and name HA  ))
  (  segid "BrD " and resid 96   and name HE% )
    2 800    2 000    2 000 peak 16532 weight  0 11000E+01 volume  0 16900E+03 ppm1     4 410 ppm2     7 607
ASSI {16692}
  (( segid "BrD " and resid 52   and name HA  ))
  (( segid "BrD " and resid 53   and name HG2 ))
    5 500    5 500    0 000 peak 16692 weight  0 11000E+01 volume  0 97221E+00 ppm1     5.592 ppm2     2 494
ASSI {16822}
  (( segid "BrD " and resid 105  and name HB1 ))
  (( segid "BrD " and resid 105  and name HA  ))
    2 600    1 700    1 700 peak 16822 weight  0 11000E+01 volume  0 25358E+03 ppm1     3 721 ppm2     4 932
ASSI {17182}
  (( segid "BrD " and resid 105  and name HB2 ))
  (( segid "BrD " and resid 105  and name HA  ))
    2 400    1 400    1 400 peak 17182 weight  0 11000E+01 volume  0.43854E+03 ppm1     3 668 ppm2     4 932
ASSI {17202}
  (( segid "BrD " and resid 105  and name HB2 ))
  (  segid "BrD " and resid 105  and name HD% )
    2.200    1 200    1.200 peak 17202 weight  0 11000E+01 volume  0 67242E+03 ppm1     3 720 ppm2     7.788
ASSI {17242}
  (( segid "BrD " and resid 105  and name HA  ))
  (  segid "BrD " and resid 105  and name HD% )
    2 200    1.200    1 200 peak 17242 weight  0 11000E+01 volume  0 69463E+03 ppm1     4 903 ppm2     7 787
ASSI {17292}
  (( segid "BrD " and resid 116  and name HA  ))
  (( segid "BrD " and resid 116  and name HG12))
    2.800    2 000    2 000 peak 17292 weight  0.11000E+01 volume  0 16843E+03 ppm1     4 804 ppm2     1 554
ASSI {17302}
  (( segid "BrD " and resid 116  and name HA  ))
  (( segid "BrD " and resid 116  and name HG11))
    3 100    2.400    2 400 peak 17302 weight  0 11000E+01 volume  0 94615E+02 ppm1     4.804 ppm2     1 917
ASSI {17412}
  (( segid "BrD " and resid 34   and name HB2 ))
  (  segid "BrD " and resid 34   and name HD% )
    2 900    2 100    2 100 peak 17412 weight  0 11000E+01 volume  0 12277E+03 ppm1     3 125 ppm2     7 705
ASSI {17652}
  (  segid "BrD " and resid 81   and name HG2%)
  (( segid "BrD " and resid 34   and name HA  ))
    2 500    1 600    1 600 peak 17652 weight  0 11000E+01 volume  0.31158E+03 ppm1     0 760 ppm2     5 542
ASSI {17662}
  (  segid "BrD " and resid 81   and name HG2%)
  (( segid "BrD " and resid 55   and name HA  ))
    2 600    1 700    1 700 peak 17662 weight  0 11000E+01 volume  0.23078E+03 ppm1     0 755 ppm2     5 366
ASSI {17722}
  (( segid "BrD " and resid 33   and name HG1 ))
  (( segid "BrD " and resid 33   and name HA  ))
    3 100    2 400    2 400 peak 17722 weight  0 11000E+01 volume  0 93743E+02 ppm1     0 859 ppm2     4 354
ASSI {17812}
  (( segid "BrD " and resid 33   and name HD2 ))
  (( segid "BrD " and resid 33   and name HB2 ))
    3 000    2 200    2 200 peak 17812 weight  0 11000E+01 volume  0 10412E+03 ppm1     2 190 ppm2    -0 162
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ASSI {17822}
  (( segid "BrD " and resid 33    and name HD1 ))
  (( segid "BrD " and resid 33    and name HB2 ))
     3 000      2 200      2 200 peak 17822 weight  0 11000E+01 volume  0 99908E+02 ppm1      2 782 ppm2      -0 162
ASSI {17832}
  (( segid "BrD " and resid 33    and name HD2 ))
  (( segid "BrD " and resid 33    and name HA  ))
     3 900      3 800      1 600 peak 17832 weight  0 11000E+01 volume  0 24295E+02 ppm1      2 190 ppm2      4.354
ASSI {17842}
  (( segid "BrD " and resid 33    and name HD1 ))
  (( segid "BrD " and resid 33    and name HA  ))
     3 800      3 600      1 700 peak 17842 weight  0 11000E+01 volume  0.26770E+02 ppm1      2 785 ppm2      4.353
ASSI {17862}
  (( segid "BrD " and resid 33    and name HD2 ))
  (( segid "BrD " and resid 32    and name HA  ))
     3.300      2 700      2 200 peak 17862 weight  0 11000E+01 volume  0 62722E+02 ppm1      2 190 ppm2      4.981
ASSI {17872}
  (( segid "BrD " and resid 33    and name HD1 ))
  (( segid "BrD " and resid 32    and name HH2 ))
     5 500      5.500      0 000 peak 17872 weight  0 11000E+01 volume  0.61193E-03 ppm1      2 783 ppm2      7 797
ASSI {17882}
  (( segid "BrD " and resid 33    and name HD2 ))
  (( segid "BrD " and resid 32    and name HH2 ))
     5 500    * 5 500      0 000 peak 17882 weight  0 11000E+01 volume  0.56139E-03 ppm1      2 191 ppm2      7 797
ASSI {17912}
  (( segid "BrD " and resid 33    and name HB1 ))
  (( segid "BrD " and resid 33    and name HD2 ))
     3 900      3 800      1 600 peak 17912 weight  0 11000E+01 volume  0 21009E+02 ppm1      1 056 ppm2      2 190
ASSI {17942}
  (( segid "BrD " and resid 33    and name HB1 ))
  (( segid "BrD " and resid 33    and name HD1 ))
     3 300      2 700      2.200 peak 17942 weight  0 11000E+01 volume  0 67464E+02 ppm1      1 056 ppm2      2 792
ASSI {18062}
  (( segid "BrD " and resid 75    and name HG1 ))
  (  segid "BrD " and resid 110   and name HG2%)
     4 000      4 000      1 500 peak 18062 weight  0 11000E+01 volume  0 20766E+02 ppm1      3 522 ppm2      1 262
ASSI {18082}
  (( segid "BrD " and resid 75    and name HG2 ))
  (  segid "BrD " and resid 110   and name HD1%)
     3 400      2 900      2 100 peak 18082 weight  0 11000E+01 volume  0 48309E+02 ppm1      3 226 ppm2      1 140
ASSI {18092}
  (( segid "BrD " and resid 75    and name HG2 ))
  (  segid "BrD " and resid 110   and name HG2%)
     4 100      4 100      1 400 peak 18092 weight  0 11000E+01 volume  0 17226E+02 ppm1      3 226 ppm2      1 262
ASSI {18162}
  (( segid "BrD " and resid 53    and name HB1 ))
  (( segid "BrD " and resid 52    and name HA  ))
     5 500      5 500      0 000 peak 18162 weight  0 11000E+01 volume  0 54558E+00 ppm1     .2 784 ppm2      5 582
ASSI {18172}
  (( segid "BrD " and resid 53    and name HB1 ))
  (  segid "BrD " and resid 46    and name HE% )
     2 600      1 700      1.700 peak 18172 weight  0 11000E+01 volume  0 27274E+03 ppm1      2 783 ppm2      6 688
ASSI {18182}
  (( segid "BrD " and resid 53    and name HB1 ))
  (  segid "BrD " and resid 47    and name HE% )
     2 500      1 600      1 600 peak 18182 weight  0.11000E+01 volume  0 34975E+03 ppm1      2 783 ppm2      7 267
ASSI {18192}
  (( segid "BrD " and resid 53    and name HA  ))
  (  segid "BrD " and resid 47    and name HD% )
     3 100      2.400      2 400 peak 18192 weight  0 11000E+01 volume  0 93621E+02 ppm1      2 777 ppm2      7 962
ASSI {18222}
  (  segid "BrD " and resid 35    and name HE% )
  (( segid "BrD " and resid 35    and name HG1 ))
     2 300      1 300      1 300 peak 18222 weight  0 11000E+01 volume  0 50180E+03 ppm1      2 781 ppm2      3 448
ASSI {18292}
  (  segid "BrD " and resid 35    and name HE% )
  (( segid "BrD " and resid 35    and name HA  ))
     2 700      1.800      1 800 peak 18292 weight  0 11000E+01 volume  0 21224E+03 ppm1      2 782 ppm2      4 901
ASSI {18452}
  (( segid "BrD " and resid 75    and name HG2 ))
  (  segid "BrD " and resid 74    and name HD% )
     3 400      2 900      2 100 peak 18452 weight  0.11000E+01 volume  0 49200E+02 ppm1      3 227 ppm2      6 999
ASSI {18462}
  (( segid "BrD " and resid 75    and name HG1 ))
  (  segid "BrD " and resid 74    and name HD% )
     3 100      2 400      2 400 peak 18462 weight  0 11000E+01 volume  0.92286E+02 ppm1      3 524 ppm2      7.001
ASSI {18512}
  (  segid "BrD " and resid 75    and name HE% )
  (( segid "BrD " and resid 75    and name HA  ))
     2 900      2 100      2 100 peak 18512 weight  0.11000E+01 volume  0 12672E+03 ppm1      2 635 ppm2      4 518
ASSI {18752}
  (  segid "BrD " and resid 75    and name HE% )
  (  segid "BrD " and resid 18    and name HD2%)
     3.800      3 600      1 700 peak 18752 weight  0 11000E+01 volume  0 27479E+02 ppm1      2 634 ppm2      0 416
ASSI {18792}
  (  segid "BrD " and resid 75    and name HE% )
  (  segid "BrD " and resid 110   and name HG2%)
     2 700      1 800      1 800 peak 18792 weight  0 11000E+01 volume  0 21856E+03 ppm1      2.634 ppm2      1.262
ASSI {18802}
  (  segid "BrD " and resid 75    and name HE% )
  (  segid "BrD " and resid 110   and name HD1%)
     2 600      1 700      1 700 peak 18802 weight  0 11000E+01 volume  0 24635E+03 ppm1      2 634 ppm2      1 140
ASSI {19032}
  (( segid "BrD " and resid 75    and name HA  ))
  (  segid "BrD " and resid 74    and name HD% )
     2.600      1.700      1.700 peak 19032 weight  0.11000E+01 volume  0.28302E+03 ppm1      4 508 ppm2      6 998
ASSI {19112}
  (  segid "BrD " and resid 43    and name HB% )
  (  segid "BrD " and resid 88    and name HE% )
     2 900      2 100      2 100 peak 19112 weight  0 11000E+01 volume  0 13802E+03 ppm1      1 700 ppm2      7 416
ASSI {19132}
  (  segid "BrD " and resid 43    and name HB% )
  (  segid "BrD " and resid 88    and name HD% )
     4.900      4 900      0 600 peak 19132 weight  0 11000E+01 volume  0 55356E+01 ppm1      1.697 ppm2      7 609
ASSI {19142}
  (  segid "BrD " and resid 43    and name HB% )
  (  segid "BrD " and resid 46    and name HE% )
     3 400      2.900      2 100 peak 19142 weight  0 11000E+01 volume  0 52712E+02 ppm1      1 697 ppm2      6 689
ASSI {19162}
  (  segid "BrD " and resid 43    and name HB% )
  (  segid "BrD " and resid 46    and name HD% )
     2 600      1 700      1 700 peak 19162 weight  0 11000E+01 volume  0 28846E+03 ppm1      1 697 ppm2      5 753
ASSI {19852}
  (( segid "BrD " and resid 102   and name HA  ))
  (( segid "BrD " and resid 102   and name HG  ))
     2 700      1 800      1 800 peak 19852 weight  0 11000E+01 volume  0 19930E+03 ppm1      4 263 ppm2      2 157
ASSI {20082}
  (( segid "BrD " and resid 110   and name HA  ))
  (( segid "BrD " and resid 110   and name HG11))
     2 400      1 400      1.400 peak 20082 weight  0 11000E+01 volume  0.38344E+03 ppm1      4.411 ppm2      1 718
ASSI {20232}
  (  segid "BrD " and resid 17    and name HG2%)
  (( segid "BrD " and resid 18    and name HA  ))
     3 100      2 400      2 400 peak 20232 weight  0 11000E+01 volume  0 91939E+02 ppm1      1 747 ppm2      3 882
ASSI {20342}
  (( segid "BrD " and resid 53    and name HA  ))
  (( segid "BrD " and resid 53    and name HD1 ))
     3 300      2 700      2.200 peak 20342 weight  0 11000E+01 volume  0 66608E+02 ppm1      4 696 ppm2      4 210
ASSI {20372}
  (( segid "BrD " and resid 53    and name HA  ))
  (  segid "BrD " and resid 47    and name HE% )
     3 900      3 800      1 600 peak 20372 weight  0 11000E+01 volume  0 22677E+02 ppm1      4 696 ppm2      7 260
ASSI {20422}
  (( segid "BrD " and resid 53    and name HD2 ))
  (( segid "BrD " and resid 53    and name HA  ))
     3 200      2 600      2 300 peak 20422 weight  0 11000E+01 volume  0 75265E+02 ppm1      4 015 ppm2      4 696
ASSI {20432}
  (( segid "BrD " and resid 53    and name HD1 ))
  (  segid "BrD " and resid 50    and name HG2%)
     3 400      2 900      2 100 peak 20432 weight  0 11000E+01 volume  0 50650E+02 ppm1      4 214 ppm2      0 993
ASSI {20462}
  (( segid "BrD " and resid 53    and name HG1 ))
  (  segid "BrD " and resid 46    and name HE% )
     3 600      3 200      1 900 peak 20462 weight  0 11000E+01 volume  0 35265E+02 ppm1      2 784 ppm2      6 689
ASSI {20472}
  (( segid "BrD " and resid 53    and name HG1 ))
  (  segid "BrD " and resid 47    and name HE% )
     2 500      1 600      1 600 peak 20472 weight  0 11000E+01 volume  0 29199E+03 ppm1      2 784 ppm2      7 267
ASSI {20482}
  (( segid "BrD " and resid 53    and name HG2 ))
  (  segid "BrD " and resid 47    and name HE% )
     2 600      1 700      1 700 peak 20482 weight  0 11000E+01 volume  0 27122E+03 ppm1      2 486 ppm2      7 267
ASSI {20492}
  (( segid "BrD " and resid 53    and name HG2 ))
  (  segid "BrD " and resid 47    and name HD% )
     2 400      1.400      1 400 peak 20492 weight  0 11000E+01 volume  0.38647E+03 ppm1      2 486 ppm2      7 958
ASSI {20502}
  (( segid "BrD " and resid 53    and name HG1 ))
  (  segid "BrD " and resid 47    and name HD% )
     2 800      2 000      2 000 peak 20502 weight  0 11000E+01 volume  0 18213E+03 ppm1      2 784 ppm2      7 958
ASSI {20522}
  (( segid "BrD " and resid 53    and name HG1 ))
  (( segid "BrD " and resid 52    and name HA  ))
     5 500      5 500      0 000 peak 20522 weight  0 11000E+01 volume  0 58337E-01 ppm1      2 784 ppm2      5 587
ASSI {20602}
  (( segid "BrD " and resid 61    and name HG2 ))
  (( segid "BrD " and resid 58    and name HA  ))
     2 500      1 600      1 600 peak 20602 weight  0 11000E+01 volume  0 31153E+03 ppm1      2 831 ppm2      4 452
ASSI {20612}
  (( segid "BrD " and resid 61    and name HG1 ))
  (( segid "BrD " and resid 58    and name HA  ))
     2.500      1 600      1 600 peak 20612 weight  0 11000E+01 volume  0 36307E+03 ppm1      2 980 ppm2      4 452
ASSI {20702}
  (( segid "BrD " and resid 80    and name HA  ))
  (( segid "BrD " and resid 83    and name HB  ))
     1 400      0 500      0 800 peak 20702 weight  0 11000E+01 volume  0 11465E+05 ppm1      4.656 ppm2      4 804
ASSI {20772}
  (( segid "BrD " and resid 58    and name HB  ))
  (( segid "BrD " and resid 54    and name HA  ))
     3 400      2 900      2 100 peak 20772 weight  0 11000E+01 volume  0 51113E+02 ppm1      4 702 ppm2      5 544
ASSI {20782}
  (  segid "BrD " and resid 58    and name HG2%)
  (( segid "BrD " and resid 54    and name HA  ))
     2 800      2.000      2 000 peak 20782 weight  0 11000E+01 volume  0 15234E+03 ppm1      1 648 ppm2      5 542
ASSI {20882}
  (( segid "BrD " and resid 62    and name HD1 ))
  (( segid "BrD " and resid 62    and name HA  ))
     3 100      2 400      2 400 peak 20882 weight  0.11000E+01 volume  0 94082E+02 ppm1      3 177 ppm2      4 476
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ASSI {20892}
  (( segid "BrD " and resid 62    and name HD2 ))
  (( segid "BrD " and resid 62    and name HA  ))
   3 000      2 200      2 200 peak 20892 weight  0 11000E+01 volume  0 10111E+03 ppm1      2 634 ppm2      4 476
ASSI {20902}
  (( segid "BrD " and resid 62    and name HD1 ))
  (  segid "BrD " and resid 67    and name HE% )
   4 400      4 400      1 100 peak 20902 weight  0 11000E+01 volume  0 11575E+02 ppm1      3 177 ppm2      7 316
ASSI {20912}
  (( segid "BrD " and resid 62    and name HD1 ))
  (  segid "BrD " and resid 67    and name HD% )
   3 700      3 400      1 800 peak 20912 weight  0 11000E+01 volume  0 30541E+02 ppm1      3 177 ppm2      6 893
ASSI {20922}
  (( segid "BrD " and resid 62    and name HD2 ))
  (  segid "BrD " and resid 67    and name HD% )
   3.400      2 900      2 100 peak 20922 weight  0 11000E+01 volume  0 54284E+02 ppm1      2.634 ppm2      6 893
ASSI {20932}
  (( segid "BrD " and resid 62    and name HD2 ))
  (  segid "BrD " and resid 67    and name HE% )
   3 100      2 400      2 400 peak 20932 weight  0 11000E+01 volume  0.91289E+02 ppm1      2 634 ppm2      7 315
ASSI {20952}
  (( segid "BrD " and resid 62    and name HB1 ))
  (( segid "BrD " and resid 62    and name HD1 ))
   3.200      2 600      2 300 peak 20952 weight  0 11000E+01 volume  0 71708E+02 ppm1      2 641 ppm2      3 183
ASSI {20962}
  (( segid "BrD " and resid 62    and name HB2 ))
  (( segid "BrD " and resid 62    and name HG1 ))
   3 000      2 200      2 200 peak 20962 weight  0 11000E+01 volume  0 10075E+03 ppm1      1 699 ppm2      2 325
ASSI {20972}
  (( segid "BrD " and resid 62    and name HG2 ))
  (( segid "BrD " and resid 62    and name HB1 ))
   2 700      1 800      1 800 peak 20972 weight  0 11000E+01 volume  0 20830E+03 ppm1      2.641 ppm2      1 479
ASSI {21012}
  (( segid "BrD " and resid 62    and name HG2 ))
  (( segid "BrD " and resid 62    and name HD1 ))
   3 100      2 400      2 400 peak 21012 weight  0 11000E+01 volume  0 87215E+02 ppm1      1 501 ppm2      3 182
ASSI {21022}
  (( segid "BrD " and resid 62    and name HG1 ))
  (( segid "BrD " and resid 62    and name HA  ))
   2 900      2 100      2 100 peak 21022 weight  0 11000E+01 volume  0 13858E+03 ppm1      2 340 ppm2      4 474
ASSI {21162}
  (( segid "BrD " and resid 83    and name HA  ))
  (( segid "BrD " and resid 86    and name HG2 ))
   4 800      4 800      0 700 peak 21162 weight  0 11000E+01 volume  0 66244E+01 ppm1      4 459 ppm2      0 766
ASSI {21512}
  (( segid "BrD " and resid 38    and name HB  ))
  (  segid "BrD " and resid 46    and name HD% )
   3 400      2 900      2 100 peak 21512 weight  0 11000E+01 volume  0.54169E+02 ppm1      1 747 ppm2      5 745
ASSI {21522}
  (( segid "BrD " and resid 38    and name HB  ))
  (  segid "BrD " and resid 47    and name HE% )
   4 500      4 500      1 000 peak 21522 weight  0 11000E+01 volume  0 90841E+01 ppm1      1 751 ppm2      7 259
ASSI {21532}
  (( segid "BrD " and resid 38    and name HB  ))
  (  segid "BrD " and resid 46    and name HE% )
   4 500      4 500      1 000 peak 21532 weight  0 11000E+01 volume  0 97356E+01 ppm1      1 747 ppm2      6 689
ASSI {21602}
  (  segid "BrD " and resid 81    and name HG1%)
  (( segid "BrD " and resid 34    and name HB2 ))
   3 300      2 700      2 200 peak 21602 weight  0.11000E+01 volume  0 56657E+02 ppm1      1 056 ppm2      3 146
ASSI {21622}
  (  segid "BrD " and resid 81    and name HG1%)
  (( segid "BrD " and resid 55    and name HA  ))
   2 400      1.400      1 400 peak 21622 weight  0 11000E+01 volume  0 44267E+03 ppm1      1 056 ppm2      5 367
ASSI {21632}
  (  segid "BrD " and resid 81    and name HG1%)
  (( segid "BrD " and resid 34    and name HA  ))
   2 800      2 000      2 000 peak 21632 weight  0 11000E+01 volume  0 15411E+03 ppm1      1 056 ppm2      5 542
ASSI {21762}
  (  segid "BrD " and resid 81    and name HG2%)
  (( segid "BrD " and resid 78    and name HA  ))
   2 600      1 700      1 700 peak 21762 weight  0 11000E+01 volume  0 24983E+03 ppm1      0 760 ppm2      4 004
ASSI {21832}
  (  segid "BrD " and resid 50    and name HD1%)
  (  segid "BrD " and resid 49    and name HG1%)
   2 900      2 100      2 100 peak 21832 weight  0 11000E+01 volume  0 14668E+03 ppm1      1 155 ppm2      1 645
ASSI {21842}
  (  segid "BrD " and resid 50    and name HD1%)
  (  segid "BrD " and resid 49    and name HG2%)
   2.400      1 400      1 400 peak 21842 weight  0.11000E+01 volume  0 37404E+03 ppm1      1 155 ppm2      1 571
ASSI {21852}
  (( segid "BrD " and resid 49    and name HB  ))
  (  segid "BrD " and resid 88    and name HD% )
   3 400      2 900      2 100 peak 21852 weight  0 11000E+01 volume  0 48521E+02 ppm1      2.634 ppm2      7 606
ASSI {21862}
  (( segid "BrD " and resid 49    and name HB  ))
  (  segid "BrD " and resid 88    and name HE% )
   3.400      2 900      2.100 peak 21862 weight  0 11000E+01 volume  0 55049E+02 ppm1      2 634 ppm2      7 414
ASSI {21872}
  (( segid "BrD " and resid 49    and name HB  ))
  (( segid "BrD " and resid 46    and name HA  ))
   3 700      3 400      1 800 peak 21872 weight  0 11000E+01 volume  0 31537E+02 ppm1      2 634 ppm2      4 143
ASSI {21912}
  (  segid "BrD " and resid 50    and name HD1%)
  (( segid "BrD " and resid 87    and name HB2 ))
   2.600      1.700      1.700 peak 21912 weight  0.11000E+01 volume  0.24085E+03 ppm1      1 155 ppm2      2 603
ASSI {21922}
  (  segid "BrD " and resid 50    and name HD1%)
  (( segid "BrD " and resid 87    and name HB1 ))
   2 400      1 400      1 400 peak 21922 weight  0 11000E+01 volume  0 36901E+03 ppm1      1 155 ppm2      2 778
ASSI {21932}
  (  segid "BrD " and resid 50    and name HD1%)
  (( segid "BrD " and resid 87    and name HG1 ))
   3.700      3 400      1 800 peak 21932 weight  0 11000E+01 volume  0 32396E+02 ppm1      1 155 ppm2      3 028
ASSI {21942}
  (  segid "BrD " and resid 50    and name HD1%)
  (( segid "BrD " and resid 84    and name HB2 ))
   2 700      1 800      1.800 peak 21942 weight  0 11000E+01 volume  0 22842E+03 ppm1      1 155 ppm2      3 272
ASSI {21962}
  (  segid "BrD " and resid 50    and name HD1%)
  (( segid "BrD " and resid 84    and name HB1 ))
   2 600      1 700      1 700 peak 21962 weight  0 11000E+01 volume  0 28478E+03 ppm1      1 155 ppm2      3 606
ASSI {21992}
  (  segid "BrD " and resid 50    and name HD1%)
  (( segid "BrD " and resid 88    and name HA  ))
   2 700      1 800      1 800 peak 21992 weight  0 11000E+01 volume  0 19153E+03 ppm1      1 155 ppm2      4.988
ASSI {22002}
  (  segid "BrD " and resid 50    and name HD1%)
  (( segid "BrD " and resid 84    and name HA  ))
   2 300      1 300      1 300 peak 22002 weight  0 11000E+01 volume  0 57384E+03 ppm1      1 155 ppm2      4 915
ASSI {22052}
  (( segid "BrD " and resid 50    and name HB  ))
  (  segid "BrD " and resid 46    and name HE% )
   3 000      2 200      2.200 peak 22052 weight  0 11000E+01 volume  0 99146E+02 ppm1      1 797 ppm2      6 689
ASSI {22092}
  (  segid "BrD " and resid 50    and name HG2%)
  (( segid "BrD " and resid 52    and name HA  ))
   3 500      3 100      2 000 peak 22092 weight  0 11000E+01 volume  0 46395E+02 ppm1      1 006 ppm2      5 587
ASSI {22102}
  (  segid "BrD " and resid 50    and name HG2%)
  (  segid "BrD " and resid 46    and name HD% )
   3 700      3 400      1.800 peak 22102 weight  0 11000E+01 volume  0 30083E+02 ppm1      1.007 ppm2      5 745
ASSI {22152}
  (  segid "BrD " and resid 50    and name HG2%)
  (  segid "BrD " and resid 47    and name HE% )
   4 300      4 300      1 200 peak 22152 weight  0 11000E+01 volume  0.12530E+02 ppm1      1.007 ppm2      7.259
ASSI {22162}
  (  segid "BrD " and resid 50    and name HG2%)
  (  segid "BrD " and resid 46    and name HE% )
   2 500      1 600      1 600 peak 22162 weight  0.11000E+01 volume  0 31318E+03 ppm1      1 007 ppm2      6 689
ASSI {22172}
  (  segid "BrD " and resid 50    and name HG2%)
  (( segid "BrD " and resid 84    and name HA  ))
   2 900      2 100      2 100 peak 22172 weight  0 11000E+01 volume  0 14754E+03 ppm1      1 007 ppm2      4 915
ASSI {22192}
  (  segid "BrD " and resid 50    and name HG2%)
  (  segid "BrD " and resid 49    and name HG2%)
   3 700      3 400      1 800 peak 22192 weight  0.11000E+01 volume  0.30274E+02 ppm1      1 006 ppm2      1.570
ASSI {22262}
  (( segid "BrD " and resid 50    and name HG12))
  (( segid "BrD " and resid 50    and name HA  ))
   3 300      2 700      2 200 peak 22262 weight  0 11000E+01 volume  0.57888E+02 ppm1      0 809 ppm2      4 522
ASSI {22342}
  (  segid "BrD " and resid 69    and name HG2%)
  (( segid "BrD " and resid 70    and name HA  ))
   3 500      3 100      2 000 peak 22342 weight  0 11000E+01 volume  0 43395E+02 ppm1      1.427 ppm2      5 356
ASSI {22512}
  (  segid "BrD " and resid 49    and name HG1%)
  (  segid "BrD " and resid 88    and name HE% )
   2 300      1 300      1.300 peak 22512 weight  0 11000E+01 volume  0.52744E+03 ppm1      1 646 ppm2      7 419
ASSI {22522}
  (  segid "BrD " and resid 49    and name HG1%)
  (  segid "BrD " and resid 88    and name HD% )
   2 500      1 600      1 600 peak 22522 weight  0 11000E+01 volume  0 29406E+03 ppm1      1 646 ppm2      7.604
ASSI {22652}
  (( segid "BrD " and resid 7     and name HG1 ))
  (( segid "BrD " and resid 7     and name HA  ))
   3 000      2 200      2 200 peak 22652 weight  0 11000E+01 volume  0.11329E+03 ppm1      2 880 ppm2      5 143
ASSI {22792}
  (( segid "BrD " and resid 104   and name HB1 ))
  (( segid "BrD " and resid 101   and name HA  ))
   2 300      1 300      1 300 peak 22792 weight  0.11000E+01 volume  0 53105E+03 ppm1      2.537 ppm2      4 267
ASSI {22872}
  (( segid "BrD " and resid 6     and name HE1 ))
  (( segid "BrD " and resid 6     and name HA  ))
   2 100      1.100      1 100 peak 22872 weight  0 11000E+01 volume  0.98321E+03 ppm1      3 610 ppm2      4 972
ASSI {22942}
  (( segid "BrD " and resid 44    and name HD2 ))
  (( segid "BrD " and resid 44    and name HA  ))
   3 100      2 400      2 400 peak 22942 weight  0.11000E+01 volume  0 83098E+02 ppm1      4 114 ppm2      5.114
ASSI {23162}
  (( segid "BrD " and resid 8     and name HG1 ))
  (( segid "BrD " and resid 8     and name HA  ))
   2 600      1 700      1 700 peak 23162 weight  0 11000E+01 volume  0 28012E+03 ppm1      2 635 ppm2      5 021
ASSI {23172}
  (( segid "BrD " and resid 11    and name HG1 ))
  (( segid "BrD " and resid 10    and name HA  ))
   4 100      4 100      1 400 peak 23172 weight  0 11000E+01 volume  0 17156E+02 ppm1      2 635 ppm2      5 477
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ASSI {23302}
  (( segid "BrD " and resid 9    and name HD1 ))
  (( segid "BrD " and resid 9    and name HA  ))
     2.900     2.100     2 100 peak 23302 weight  0 11000E+01 volume  0 13154E+03 ppm1     3 768 ppm2     4 940
ASSI {23352}
  (( segid "BrD " and resid 9    and name HD1 ))
  (( segid "BrD " and resid 9    and name HB1 ))
     2 400     1 400     1 400 peak 23352 weight  0 11000E+01 volume  0 39945E+03 ppm1     3 768 ppm2     2 434
ASSI {23362}
  (( segid "BrD " and resid 9    and name HD1 ))
  (( segid "BrD " and resid 9    and name HB2 ))
     2 300     1.300     1 300 peak 23362 weight  0 11000E+01 volume  0 50335E+03 ppm1     3.768 ppm2     2 385
ASSI {23542}
  (( segid "BrD " and resid 11   and name HA  ))
  (( segid "BrD " and resid 11   and name HD1 ))
     2 600     1 700     1 700 peak 23542 weight  0 11000E+01 volume  0 23295E+03 ppm1     4.951 ppm2     4 459
ASSI {23552}
  (  segid "BrD " and resid 14   and name HD2%)
  (( segid "BrD " and resid 11   and name HA  ))
     2 500     1 600     1.600 peak 23552 weight  0 11000E+01 volume  0 34571E+03 ppm1     1 401 ppm2     4 947
ASSI {23692}
  (( segid "BrD " and resid 14   and name HB2 ))
  (  segid "BrD " and resid 18   and name HD1%)
     2 900     2 100     2 100 peak 23692 weight  0.11000E+01 volume  0 14113E+03 ppm1     2 143 ppm2     1 084
ASSI {23702}
  (( segid "BrD " and resid 14   and name HA  ))
  (  segid "BrD " and resid 17   and name HG2%)
     3 400     2.900     2 100 peak 23702 weight  0 11000E+01 volume  0 49626E+02 ppm1     4 656 ppm2     1 750
ASSI {23722}
  (( segid "BrD " and resid 14   and name HG  ))
  (  segid "BrD " and resid 18   and name HD2%)
     3 200     2 600     2 300 peak 23722 weight  0 11000E+01 volume  0 69871E+02 ppm1     2 044 ppm2     0 415
ASSI {23752}
  (( segid "BrD " and resid 14   and name HA  ))
  (( segid "BrD " and resid 17   and name HB  ))
     2 100     1 100     1 100 peak 23752 weight  0.11000E+01 volume  0 89711E+03 ppm1     4 656 ppm2     4 854
ASSI {23852}
  (  segid "BrD " and resid 14   and name HD1%)
  (( segid "BrD " and resid 11   and name HA  ))
     2 200     1 200     1 200 peak 23852 weight  0 11000E+01 volume  0 75160E+03 ppm1     1 402 ppm2     4 947
ASSI {23952}
  (( segid "BrD " and resid 18   and name HB2 ))
  (( segid "BrD " and resid 15   and name HA  ))
     3.200     2 600     2 300 peak 23952 weight  0 11000E+01 volume  0 79651E+02 ppm1     0 911 ppm2     4 630
ASSI {23962}
  (( segid "BrD " and resid 18   and name HB1 ))
  (( segid "BrD " and resid 15   and name HA  ))
     3 100     2.400     2 400 peak 23962 weight  0 11000E+01 volume  0 98332E+02 ppm1     2 144 ppm2     4 626
ASSI {24042}
  (  segid "BrD " and resid 18   and name HD2%)
  (( segid "BrD " and resid 17   and name HB  ))
     2 900     2 100     2 100 peak 24042 weight  0 11000E+01 volume  0 13399E+03 ppm1     0 414 ppm2     4 860
ASSI {24052}
  (  segid "BrD " and resid 18   and name HD2%)
  (  segid "BrD " and resid 74   and name HD% )
     2 500     1 600     1 600 peak 24052 weight  0 11000E+01 volume  0 29789E+03 ppm1     0 415 ppm2     6 998
ASSI {24062}
  (  segid "BrD " and resid 18   and name HD2%)
  (  segid "BrD " and resid 74   and name HE% )
     2 700     1.800     1 800 peak 24062 weight  0 11000E+01 volume  0 22219E+03 ppm1     0 415 ppm2     7 534
ASSI {24072}
  (  segid "BrD " and resid 18   and name HD2%)
  (( segid "BrD " and resid 74   and name HB1 ))
     3 200     2 600     2 300 peak 24072 weight  0 11000E+01 volume  0.70185E+02 ppm1     0 419 ppm2     3 565
ASSI {24082}
  (  segid "BrD " and resid 18   and name HD2%)
  (( segid "BrD " and resid 74   and name HB2 ))
     2 900     2.100     2 100 peak 24082 weight  0 11000E+01 volume  0 13658E+03 ppm1     0 415 ppm2     2 995
ASSI {24092}
  (  segid "BrD " and resid 18   and name HD2%)
  (  segid "BrD " and resid 63   and name HD1%)
     3 200     2 600     2 300 peak 24092 weight  0 11000E+01 volume  0 72579E+02 ppm1     0.414 ppm2     1 648
ASSI {24132}
  (  segid "BrD " and resid 18   and name HD2%)
  (( segid "BrD " and resid 74   and name HA  ))
     3 400     2 900     2 100 peak 24132 weight  0 11000E+01 volume  0 52592E+02 ppm1     0 414 ppm2     4 378
ASSI {24162}
  (  segid "BrD " and resid 18   and name HD1%)
  (  segid "BrD " and resid 74   and name HE% )
     3 000     2 200     2 200 peak 24162 weight  0 11000E+01 volume  0 10145E+03 ppm1     1.058 ppm2     7 536
ASSI {24182}
  (  segid "BrD " and resid 18   and name HD1%)
  (  segid "BrD " and resid 74   and name HD% )
     2 600     1.700     1 700 peak 24182 weight  0 11000E+01 volume  0 27877E+03 ppm1     1 056 ppm2     6.998
ASSI {24212}
  (  segid "BrD " and resid 18   and name HD1%)
  (( segid "BrD " and resid 74   and name HA  ))
     3 200     2.600     2 300 peak 24212 weight  0 11000E+01 volume  0 78587E+02 ppm1     1 056 ppm2     4 378
ASSI {24522}
  (  segid "BrD " and resid 63   and name HD1%)
  (( segid "BrD " and resid 19   and name HA  ))
     2 600     1.700     1 700 peak 24522 weight  0 11000E+01 volume  0 26998E+03 ppm1     1 647 ppm2     4 297
ASSI {24662}
  (  segid "BrD " and resid 63   and name HD2%)
  (  segid "BrD " and resid 18   and name HD1%)
     2.700     1.800     1.800 peak 24662 weight  0.11000E+01 volume  0.19359E+03 ppm1     1 498 ppm2     1 090
ASSI {24672}
  (  segid "BrD " and resid 63   and name HD2%)
  (( segid "BrD " and resid 18   and name HB2 ))
     5 500     5 500     0 000 peak 24672 weight  0 11000E+01 volume  0 20841E+01 ppm1     1.498 ppm2     0 925
ASSI {24742}
  (( segid "BrD " and resid 19   and name HB2 ))
  (( segid "BrD " and resid 19   and name HE1 ))
     4 000     4.000     1.500 peak 24742 weight  0 11000E+01 volume  0 20066E+02 ppm1     1 989 ppm2     3 525
ASSI {24752}
  (( segid "BrD " and resid 19   and name HB1 ))
  (( segid "BrD " and resid 19   and name HE1 ))
     3 300     2 700     2 200 peak 24752 weight  0 11000E+01 volume  0 65557E+02 ppm1     2 290 ppm2     3 525
ASSI {24762}
  (( segid "BrD " and resid 19   and name HG1 ))
  (( segid "BrD " and resid 16   and name HA  ))
     2 900     2 100     2 100 peak 24762 weight  0 11000E+01 volume  0 12763E+03 ppm1     1.894 ppm2     4 508
ASSI {24812}
  (( segid "BrD " and resid 19   and name HD1 ))
  (( segid "BrD " and resid 16   and name HA  ))
     2 300     1 300     1 300 peak 24812 weight  0 11000E+01 volume  0 50116E+03 ppm1     2 192 ppm2     4 507
ASSI {24872}
  (( segid "BrD " and resid 23   and name HG1 ))
  (( segid "BrD " and resid 20   and name HA  ))
     3 100     2 400     2 400 peak 24872 weight  0 11000E+01 volume  0 91712E+02 ppm1     3 124 ppm2     4 893
ASSI {24902}
  (( segid "BrD " and resid 24   and name HG1 ))
  (( segid "BrD " and resid 21   and name HA  ))
     3.200     2 600     2 300 peak 24902 weight  0 11000E+01 volume  0 67606E+02 ppm1     3 469 ppm2     4 370
ASSI {24912}
  (( segid "BrD " and resid 24   and name HG2 ))
  (( segid "BrD " and resid 21   and name HA  ))
     2 600     1 700     1 700 peak 24912 weight  0 11000E+01 volume  0 26410E+03 ppm1     3 076 ppm2     4 370
ASSI {24932}
  (( segid "BrD " and resid 24   and name HA  ))
  (( segid "BrD " and resid 24   and name HB1 ))
     2 200     1 200     1 200 peak 24932 weight  0 11000E+01 volume  0.62910E+03 ppm1     4 784 ppm2     3 074
ASSI {25432}
  (( segid "BrD " and resid 85   and name HB1 ))
  (( segid "BrD " and resid 82   and name HA  ))
     3 100     2.400     2 400 peak 25432 weight  0 11000E+01 volume  0 87929E+02 ppm1     3 917 ppm2     4 753
ASSI {25552}
  (( segid "BrD " and resid 101  and name HG12))
  (( segid "BrD " and resid 101  and name HB  ))
     2 300     1 300     1 300 peak 25552 weight  0.11000E+01 volume  0 55437E+03 ppm1     1 797 ppm2     2 538
ASSI {25612}
  (  segid "BrD " and resid 21   and name HG2%)
  (( segid "BrD " and resid 18   and name HA  ))
     3 000     2.200     2 200 peak 25612 weight  0 11000E+01 volume  0 11187E+03 ppm1     1 599 ppm2     3 890
ASSI {26032}
  (  segid "BrD " and resid 110  and name HD1%)
  (( segid "BrD " and resid 75   and name HG1 ))
     3 400     2 900     2 100 peak 26032 weight  0.11000E+01 volume  0 51048E+02 ppm1     1.155 ppm2     3 524
ASSI {26172}
  (  segid "BrD " and resid 110  and name HG2%)
  (  segid "BrD " and resid 18   and name HD2%)
     4 400     4 400     1.100 peak 26172 weight  0 11000E+01 volume  0.11733E+02 ppm1     1 254 ppm2     0 408
ASSI {26182}
  (  segid "BrD " and resid 110  and name HD1%)
  (  segid "BrD " and resid 18   and name HD2%)
     3.000     2 200     2 200 peak 26182 weight  0 11000E+01 volume  0 11735E+03 ppm1     1 153 ppm2     0.410
ASSI {26302}
  (  segid "BrD " and resid 116  and name HD1%)
  (( segid "BrD " and resid 116  and name HA  ))
     2 500     1.600     1 600 peak 26302 weight  0 11000E+01 volume  0 31414E+03 ppm1     1 401 ppm2     4 826
ASSI {26562}
  (( segid "BrD " and resid 103  and name HA  ))
  (  segid "BrD " and resid 106  and name HD% )
     3 100     2 400     2.400 peak 26562 weight  0 11000E+01 volume  0 97052E+02 ppm1     3 768 ppm2     7 514
ASSI {26592}
  (( segid "BrD " and resid 103  and name HB1 ))
  (( segid "BrD " and resid 100  and name HA  ))
     2 700     1.800     1 800 peak 26592 weight  0.11000E+01 volume  0 20226E+03 ppm1     2 338 ppm2     4 946
ASSI {26642}
  (( segid "BrD " and resid 103  and name HB2 ))
  (( segid "BrD " and resid 103  and name HG2 ))
     2.000     1 000     1.000 peak 26642 weight  0.11000E+01 volume  0.14101E+04 ppm1     1 893 ppm2     2 520
ASSI {26652}
  (( segid "BrD " and resid 103  and name HB2 ))
  (( segid "BrD " and resid 103  and name HG1 ))
     2 200     1 200     1 200 peak 26652 weight  0.11000E+01 volume  0 62174E+03 ppm1     1 893 ppm2     2 598
ASSI {26662}
  (( segid "BrD " and resid 103  and name HG2 ))
  (( segid "BrD " and resid 100  and name HA  ))
     3 500     3 100     2.000 peak 26662 weight  0 11000E+01 volume  0 45243E+02 ppm1     2 519 ppm2     4.947
ASSI {26672}
  (( segid "BrD " and resid 103  and name HG1 ))
  (( segid "BrD " and resid 100  and name HA  ))
     3 900     3.800     1 600 peak 26672 weight  0 11000E+01 volume  0 23440E+02 ppm1     2.598 ppm2     4.947
ASSI {26722}
  (( segid "BrD " and resid 94   and name HG1 ))
  (( segid "BrD " and resid 32   and name HH2 ))
     2 900     2 100     2 100 peak 26722 weight  0 11000E+01 volume  0 14855E+03 ppm1     3.129 ppm2     7 788
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ASSI {26782}
  (( segid "BrD " and resid 94   and name HB1 ))
  (( segid "BrD " and resid 32   and name HZ2 ))
     2 500     1 600     1 600 peak 26782 weight  0 11000E+01 volume  0 35938E+03 ppm1     2 735 ppm3     7 998
ASSI {26792}
  (( segid "BrD " and resid 94   and name HB1 ))
  (( segid "BrD " and resid 32   and name HH2 ))
     3 000     2.200     2 200 peak 26792 weight  0 11000E+01 volume  0 10089E+03 ppm1     2 733 ppm2     7 785
ASSI {26842}
  (( segid "BrD " and resid 94   and name HG1 ))
  (( segid "BrD " and resid 94   and name HB1 ))
     2 200     1 200     1 200 peak 26842 weight  0 11000E+01 volume  0.72439E+03 ppm1     3 123 ppm2     2 731
ASSI {26862}
  (( segid "BrD " and resid 87   and name HG2 ))
  (( segid "BrD " and resid 86   and name HD1 ))
     3 600     3 200     1.900 peak 26862 weight  0 11000E+01 volume  0 34874E+02 ppm1     2 782 ppm2     1 900
ASSI {26882}
  (( segid "BrD " and resid 87   and name HB1 ))
  (( segid "BrD " and resid 87   and name HG1 ))
     2 400     1 400     1 400 peak 26882 weight  0 11000E+01 volume  0 47090E+03 ppm1     2 779 ppm2     3 021
ASSI {27152}
  (( segid "BrD " and resid 80   and name HD2 ))
  (( segid "BrD " and resid 80   and name HA  ))
     2 400     1 400     1.400 peak 27152 weight  0 11000E+01 volume  0 41973E+03 ppm1     3 912 ppm2     4 678
ASSI {27162}
  (( segid "BrD " and resid 80   and name HD1 ))
  (( segid "BrD " and resid 80   and name HA  ))
     2.600     1 700     1 700 peak 27162 weight  0 11000E+01 volume  0 27730E+03 ppm1     3 962 ppm2     4 677
ASSI {27212}
  (( segid "BrD " and resid 77   and name HB1 ))
  (( segid "BrD " and resid 74   and name HA  ))
     2 800     2 000     2 000 peak 27212 weight  0 11000E+01 volume  0 16302E+03 ppm1     3 325 ppm2     4 378
ASSI {27242}
  (( segid "BrD " and resid 80   and name HB2 ))
  (( segid "BrD " and resid 80   and name HD1 ))
     2 900     2 100     2 100 peak 27242 weight  0 11000E+01 volume  0 12614E+03 ppm1     2 536 ppm2     3 955
ASSI {27252}
  (( segid "BrD " and resid 80   and name HB2 ))
  (( segid "BrD " and resid 80   and name HD2 ))
     2 800     2 000     2 000 peak 27252 weight  0 11000E+01 volume  0 14981E+03 ppm1     2 536 ppm2     3 890
ASSI {27312}
  (( segid "BrD " and resid 56   and name HG  ))
  (( segid "BrD " and resid 34   and name HA  ))
     5 500     5 500     0 000 peak 27312 weight  0 11000E+01 volume  0 47841E+00 ppm1     2 338 ppm2     5 542
ASSI {27352}
  (( segid "BrD " and resid 55   and name HB1 ))
  (( segid "BrD " and resid 55   and name HA  ))
     2 200     1 200     1 200 peak 27352 weight  0 11000E+01 volume  0 72273E+03 ppm1     2 979 ppm2     5 366
ASSI {27412}
  (  segid "BrD " and resid 81   and name HG1%)
  (( segid "BrD " and resid 34   and name HB1 ))
     3 100     2.400     2 400 peak 27412 weight  0 11000E+01 volume  0 93003E+02 ppm1     1 058 ppm2     4 106
ASSI {27512}
  (  segid "BrD " and resid 22   and name HD2%)
  (( segid "BrD " and resid 22   and name HG  ))
     1 900     0 900     0.900 peak 27512 weight  0 11000E+01 volume  0 14735E+04 ppm1     1 599 ppm2     2 362
ASSI {27522}
  (  segid "BrD " and resid 22   and name HD2%)
  (( segid "BrD " and resid 22   and name HB2 ))
     2 200     1 200     1 200 peak 27522 weight  0 11000E+01 volume  0.70123E+03 ppm1     1 599 ppm2     2.286
ASSI {27682}
  (  segid "BrD " and resid 73   and name HD2%)
  (( segid "BrD " and resid 73   and name HB2 ))
     2 900     2 100     2 100 peak 27682 weight  0.11000E+01 volume  0 12667E+03 ppm1     1 600 ppm2     2 483
ASSI {27922}
  (  segid "BrD " and resid 78   and name HD1%)
  (  segid "BrD " and resid 82   and name HD% )
     3 600     3 200     1 900 peak 27922 weight  0 11000E+01 volume  0 39776E+02 ppm1     0 760 ppm2     7.259
ASSI {27972}
  (  segid "BrD " and resid 78   and name HD2%)
  (  segid "BrD " and resid 82   and name HD% )
     3 400     2 900     2 100 peak 27972 weight  0 11000E+01 volume  0 49710E+02 ppm1     0 662 ppm2     7 259
ASSI {28242}
  (  segid "BrD " and resid 56   and name HD1%)
  (( segid "BrD " and resid 34   and name HB1 ))
     3.000     2 200     2 200 peak 28242 weight  0 11000E+01 volume  0.10505E+03 ppm1     1 549 ppm2     4 110
ASSI {28282}
  (  segid "BrD " and resid 56   and name HD2%)
  (( segid "BrD " and resid 34   and name HA  ))
     3 800     3.600     1.700 peak 28282 weight  0 11000E+01 volume  0.25930E+02 ppm1     1 253 ppm2     5 540
ASSI {28312}
  (  segid "BrD " and resid 56   and name HD2%)
  (( segid "BrD " and resid 34   and name HB1 ))
     3 400     2.900     2.100 peak 28312 weight  0 11000E+01 volume  0 48455E+02 ppm1     1 253 ppm2     4 110
ASSI {28362}
  (  segid "BrD " and resid 56   and name HD2%)
  (( segid "BrD " and resid 34   and name HB2 ))
     3.200     2 600     2 300 peak 28362 weight  0 11000E+01 volume  0.68625E+02 ppm1     1 254 ppm2     3 134
ASSI {28672}
  (  segid "BrD " and resid 102  and name HD1%)
  (( segid "BrD " and resid 102  and name HA  ))
     2 100     1.100     1 100 peak 28672 weight  0 11000E+01 volume  0 89519E+03 ppm1     1 303 ppm2     4 282
ASSI {28712}
  (  segid "BrD " and resid 102  and name HD2%)
  (( segid "BrD " and resid 102  and name HB2 ))
     2.000     1.000     1.000 peak 28712 weight  0.11000E+01 volume  0.12274E+04 ppm1     1.303 ppm2     1 832
ASSI {28802}
  (( segid "BrD " and resid 115  and name HG  ))
  (( segid "BrD " and resid 115  and name HA  ))
     2 400     1 400     1 400 peak 28802 weight  0 11000E+01 volume  0 40182E+03 ppm1     2.143 ppm2     4 828
ASSI {28962}
  (  segid "BrD " and resid 56   and name HD1%)
  (( segid "BrD " and resid 34   and name HA  ))
     3 200     2 600     2 300 peak 28962 weight  0.11000E+01 volume  0 68400E+02 ppm1     1 544 ppm2     5 540
ASSI {28982}
  (( segid "BrD " and resid 59   and name HG2 ))
  (( segid "BrD " and resid 56   and name HA  ))
     2.400     1 400     1 400 peak 28982 weight  0.11000E+01 volume  0 37484E+03 ppm1     3 137 ppm2     4 636
ASSI {29062}
  (  segid "BrD " and resid 59   and name HE% )
  (( segid "BrD " and resid 56   and name HA  ))
     3.100     2 400     2 400 peak 29062 weight  0 11000E+01 volume  0 84530E+02 ppm1     1 847 ppm2     4 636
ASSI {29122}
  (  segid "BrD " and resid 59   and name HE% )
  (  segid "BrD " and resid 74   and name HE% )
     2 400     1 400     1 400 peak 29122 weight  0 11000E+01 volume  0.44730E+03 ppm1     1 848 ppm2     7 535
ASSI {29182}
  (  segid "BrD " and resid 54   and name HE% )
  (( segid "BrD " and resid 58   and name HB  ))
     3 000     2 200     2 200 peak 29182 weight  0 11000E+01 volume  0 12060E+03 ppm1     2 536 ppm2     4 696
ASSI {29282}
  (( segid "BrD " and resid 54   and name HB1 ))
  (( segid "BrD " and resid 54   and name HG1 ))
     2 800     2 000     2 000 peak 29282 weight  0 11000E+01 volume  0.16180E+03 ppm1     2 585 ppm2     3 304
ASSI {29312}
  (( segid "BrD " and resid 44   and name HB2 ))
  (( segid "BrD " and resid 44   and name HD2 ))
     3 500     3 100     2 000 peak 29312 weight  0 11000E+01 volume  0 45332E+02 ppm1     2 634 ppm2     4 126
ASSI {29342}
  (( segid "BrD " and resid 44   and name HG2 ))
  (( segid "BrD " and resid 43   and name HA  ))
     3 600     3 200     1 900 peak 29342 weight  0 11000E+01 volume  0 36619E+02 ppm1     2 645 ppm2     5 542
ASSI {29362}
  (( segid "BrD " and resid 44   and name HD1 ))
  (( segid "BrD " and resid 44   and name HA  ))
     3 200     2 600     2 300 peak 29362 weight  0 11000E+01 volume  0 69345E+02 ppm1     4 310 ppm2     5 114
ASSI {29422}
  (( segid "BrD " and resid 91   and name HB1 ))
  (( segid "BrD " and resid 91   and name HD2 ))
     2 600     1 700     1 700 peak 29422 weight  0 11000E+01 volume  0 26299E+03 ppm1     2 978 ppm2     4 407
ASSI {29432}
  (( segid "BrD " and resid 91   and name HB2 ))
  (( segid "BrD " and resid 91   and name HD2 ))
     2 800     2 000     2 000 peak 29432 weight  0 11000E+01 volume  0 15191E+03 ppm1     2 730 ppm2     4 407
ASSI {29492}
  (( segid "BrD " and resid 79   and name HG1 ))
  (( segid "BrD " and resid 76   and name HA  ))
     2 400     1 400     1 400 peak 29492 weight  0.11000E+01 volume  0 46894E+03 ppm1     3 033 ppm2     4 680
ASSI {29612}
  (( segid "BrD " and resid 70   and name HA  ))
  (  segid "BrD " and resid 69   and name HG1%)
     4.000     4 000     1 500 peak 29612 weight  0 11000E+01 volume  0 20014E+02 ppm1     5 346 ppm2     1 547
ASSI {29932}
  (( segid "BrD " and resid 66   and name HB2 ))
  (( segid "BrD " and resid 66   and name HD2 ))
     2 700     1 800     1 800 peak 29932 weight  0 11000E+01 volume  0 20564E+03 ppm1     2 641 ppm2     3 633
ASSI {29942}
  (( segid "BrD " and resid 66   and name HB1 ))
  (( segid "BrD " and resid 66   and name HD2 ))
     2 600     1 700     1 700 peak 29942 weight  0.11000E+01 volume  0 23040E+03 ppm1     2 701 ppm2     3 636
ASSI {29952}
  (( segid "BrD " and resid 66   and name HB2 ))
  (( segid "BrD " and resid 66   and name HD1 ))
     2 600     1 700     1 700 peak 29952 weight  0 11000E+01 volume  0.23393E+03 ppm1     2 633 ppm2     3 670
ASSI {29962}
  (( segid "BrD " and resid 66   and name HB1 ))
  (( segid "BrD " and resid 66   and name HD1 ))
     2 700     1 800     1 800 peak 29962 weight  0 11000E+01 volume  0 22124E+03 ppm1     2 701 ppm2     3 669
ASSI {30032}
  (( segid "BrD " and resid 51   and name HA  ))
  (( segid "BrD " and resid 52   and name HA  ))
     4 100     4 100     1 400 peak 30032 weight  0 11000E+01 volume  0 17278E+02 ppm1     4 459 ppm2     5 585
ASSI {30052}
  (( segid "BrD " and resid 86   and name HD1 ))
  (( segid "BrD " and resid 86   and name HA  ))
     3 500     3 100     2 000 peak 30052 weight  0 11000E+01 volume  0 45287E+02 ppm1     1 895 ppm2     4.810
ASSI {30162}
  (( segid "BrD " and resid 64   and name HA  ))
  (  segid "BrD " and resid 15   and name HE% )
     2 400     1 400     1 400 peak 30162 weight  0.11000E+01 volume  0 39658E+03 ppm1     4 950 ppm2     7 485
ASSI {30202}
  (( segid "BrD " and resid 64   and name HE1 ))
  (( segid "BrD " and resid 64   and name HA  ))
     2 300     1.300     1 300 peak 30202 weight  0 11000E+01 volume  0.49260E+03 ppm1     3.597 ppm2     4 939
ASSI {30342}
  (( segid "BrD " and resid 86   and name HB1 ))
  (  segid "BrD " and resid 96   and name HD% )
     2 700     1 800     1 800 peak 30342 weight  0 11000E+01 volume  0.18798E+03 ppm1     2 337 ppm2     7 722
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ASSI {30352}
  (( segid "BrD " and resid 86    and name HB1 ))
  (  segid "BrD " and resid 96    and name HE% )
     2.700     1 800     1 800 peak 30352 weight  0 11000E+01 volume  0 21345E+03 ppm1      2 338 ppm2      7 603
ASSI {30392}
  (( segid "BrD " and resid 86    and name HE1 ))
  (( segid "BrD " and resid 86    and name HA  ))
     3 100     2 400     2 400 peak 30392 weight  0 11000E+01 volume  0 90505E+02 ppm1      3 080 ppm2      4 808
ASSI {30402}
  (( segid "BrD " and resid 86    and name HE1 ))
  (( segid "BrD " and resid 86    and name HB1 ))
     2 200     1 200     1 200 peak 30402 weight  0.11000E+01 volume  0 64111E+03 ppm1      3 079 ppm2      2 370
ASSI {30412}
  (( segid "BrD " and resid 86    and name HE1 ))
  (( segid "BrD " and resid 86    and name HG1 ))
     2 900     2 100     2.100 peak 30412 weight  0 11000E+01 volume  0 14017E+03 ppm1      3 079 ppm2      1.896
ASSI {30512}
  (( segid "BrD " and resid 109   and name HE1 ))
  (( segid "BrD " and resid 109   and name HA  ))
     2 900     2 100     2 100 peak 30512 weight  0 11000E+01 volume  0 12187E+03 ppm1      3 176 ppm2      4 639
ASSI {30522}
  (( segid "BrD " and resid 109   and name HD1 ))
  (( segid "BrD " and resid 109   and name HA  ))
     1 900     0 900     0 900 peak 30522 weight  0 11000E+01 volume  0 17943E+04 ppm1      1 994 ppm2      4 639
ASSI {30622}
  (( segid "BrD " and resid 109   and name HB1 ))
  (( segid "BrD " and resid 106   and name HA  ))
     2.400     1 400     1 400 peak 30622 weight  0 11000E+01 volume  0 44758E+03 ppm1      2 334 ppm2      4 575
ASSI {30632}
  (( segid "BrD " and resid 109   and name HB2 ))
  (( segid "BrD " and resid 106   and name HA  ))
     2 700     1 800     1 800 peak 30632 weight  0 11000E+01 volume  0.21060E+03 ppm1      2 139 ppm2      4 573
ASSI {30732}
  (( segid "BrD " and resid 97    and name HG2 ))
  (( segid "BrD " and resid 97    and name HA  ))
     2 400     1 400     1 400 peak 30732 weight  0 11000E+01 volume  0 42305E+03 ppm1      2 143 ppm2      4 800
ASSI {30802}
  (( segid "BrD " and resid 104   and name HD1 ))
  (( segid "BrD " and resid 104   and name HA  ))
     1.700     0 700     0 700 peak 30802 weight  0 11000E+01 volume  0.32351E+04 ppm1      2 289 ppm2      4.671
ASSI {30862}
  (( segid "BrD " and resid 111   and name HG1 ))
  (( segid "BrD " and resid 111   and name HA  ))
     2 500     1 600     1 600 peak 30862 weight  0 11000E+01 volume  0 32568E+03 ppm1      2 000 ppm2      4 670
ASSI {30872}
  (( segid "BrD " and resid 111   and name HD1 ))
  (( segid "BrD " and resid 111   and name HA  ))
     2 500     1 600     1.600 peak 30872 weight  0 11000E+01 volume  0 34175E+03 ppm1      2 240 ppm2      4 656
ASSI {30912}
  (( segid "BrD " and resid 111   and name HE1 ))
  (( segid "BrD " and resid 111   and name HA  ))
     2 200     1 200     1 200 peak 30912 weight  0 11000E+01 volume  0 72636E+03 ppm1      3 520 ppm2      4 656
ASSI {31022}
  (( segid "BrD " and resid 72    and name HD1 ))
  (( segid "BrD " and resid 72    and name HE2 ))
     2 200     1 200     1 200 peak 31022 weight  0 11000E+01 volume  0 72521E+03 ppm1      2 287 ppm2      3 654
ASSI {31032}
  (( segid "BrD " and resid 72    and name HD1 ))
  (( segid "BrD " and resid 72    and name HE1 ))
     2 300     1 300     1 300 peak 31032 weight  0 11000E+01 volume  0 50216E+03 ppm1      2 287 ppm2      3 744
ASSI {31042}
  (( segid "BrD " and resid 72    and name HB1 ))
  (( segid "BrD " and resid 72    and name HE1 ))
     2 200     1 200     1 200 peak 31042 weight  0.11000E+01 volume  0 79378E+03 ppm1      2 387 ppm2      3.744
ASSI {31052}
  (( segid "BrD " and resid 72    and name HB1 ))
  (( segid "BrD " and resid 72    and name HE2 ))
     1 900     0 900     0 900 peak 31052 weight  0 11000E+01 volume  0 15518E+04 ppm1      2 386 ppm2      3 652
ASSI { 1632}
  (  segid "BrD " and resid 110   and name HD1%)
  (( segid "BrD " and resid 78    and name HB1 ))
     2 100     2 100     2 400 peak  1632 weight  0.10000E+01 volume  0 10163E+04 ppm1      1 154 ppm2      1 309
ASSI { 4042}
  (( segid "BrD " and resid 79    and name HG1 ))
  (( segid "BrD " and resid 80    and name HG1 ))
     3.700     3 400     1 800 peak  4042 weight  0 10000E+01 volume  0 30439E+02 ppm1      3 029 ppm2      2 351
ASSI { 4882}
  (( segid "BrD " and resid 19    and name HD1 ))
  (  segid "BrD " and resid 63    and name HD2%)
     2 700     1 800     1 800 peak  4882 weight  0 10000E+01 volume  0 22363E+03 ppm1      2 191 ppm2      1 495
ASSI { 4902}
  (( segid "BrD " and resid 97    and name HB1 ))
  (  segid "BrD " and resid 101   and name HD1%)
     3 000     2 200     2.200 peak  4902 weight  0 10000E+01 volume  0 10809E+03 ppm1      2 683 ppm2      1 580
ASSI { 4992}
  (( segid "BrD " and resid 37    and name HG2 ))
  (( segid "BrD " and resid 55    and name HA  ))
     4 200     4 200     1 300 peak  4992 weight  0 10000E+01 volume  0 14817E+02 ppm1      2 586 ppm2      5.380
ASSI { 6092}
  (( segid "BrD " and resid 115   and name HG  ))
  (  segid "BrD " and resid 110   and name HG2%)
     3 700     3 400     1 800 peak  6092 weight  0 10000E+01 volume  0 29496E+02 ppm1      2 140 ppm2      1 222
ASSI { 6222}
  (  segid "BrD " and resid 22    and name HD2%)
  (  segid "BrD " and resid 56    and name HD2%)
     2.300     1.300     1.300 peak  6222 weight  0 10000E+01 volume  0 52799E+03 ppm1      1.599 ppm2      1 246
ASSI { 6602}
  (  segid "BrD " and resid 31    and name HB% )
  (  segid "BrD " and resid 56    and name HD1%)
     2 500     1.600     1.600 peak  6602 weight  0 10000E+01 volume  0 34161E+03 ppm1      2 291 ppm2      1.539
ASSI { 6792}
  (  segid "BrD " and resid 99    and name HB% )
  (( segid "BrD " and resid 82    and name HA  ))
     3 000     2.200     2 200 peak  6792 weight  0 10000E+01 volume  0 12038E+03 ppm1      2 190 ppm2      4 752
ASSI { 6832}
  (  segid "BrD " and resid 99    and name HB% )
  (( segid "BrD " and resid 86    and name HG2 ))
     3 000     2 200     2 200 peak  6832 weight  0 10000E+01 volume  0 11935E+03 ppm1      2 191 ppm2      0 765
ASSI { 6852}
  (  segid "BrD " and resid 113   and name HB% )
  (  segid "BrD " and resid 110   and name HG2%)
     2.800     2 000     2 000 peak  6852 weight  0 10000E+01 volume  0 15622E+03 ppm1      1 991 ppm2      1.221
ASSI { 6862}
  (  segid "BrD " and resid 113   and name HB% )
  (  segid "BrD " and resid 18    and name HD1%)
     4 900     4.900     0 600 peak  6862 weight  0 10000E+01 volume  0 56980E+01 ppm1      1 991 ppm2      1.066
ASSI { 6902}
  (( segid "BrD " and resid 31    and name HA  ))
  (( segid "BrD " and resid 33    and name HD1 ))
     3 300     2 700     2 200 peak  6902 weight  0 10000E+01 volume  0 60152E+02 ppm1      5 000 ppm2      2 794
ASSI { 6952}
  (  segid "BrD " and resid 25    and name HG2%)
  (  segid "BrD " and resid 31    and name HB% )
     2 500     1.600     1 600 peak  6952 weight  0 10000E+01 volume  0 32952E+03 ppm1      1 650 ppm2      2 320
ASSI { 6982}
  (  segid "BrD " and resid 25    and name HG2%)
  (  segid "BrD " and resid 56    and name HD2%)
     2 500     1 600     1 600 peak  6982 weight  0 10000E+01 volume  0.36117E+03 ppm1      1 646 ppm2      1 252
ASSI { 7362}
  (  segid "BrD " and resid 25    and name HG2%)
  (( segid "BrD " and resid 102   and name HG  ))
     2 900     2 100     2 100 peak  7362 weight  0 10000E+01 volume  0 13044E+03 ppm1      1 647 ppm2      2 157
ASSI { 7412}
  (( segid "BrD " and resid 46    and name HA  ))
  (  segid "BrD " and resid 49    and name HG1%)
     3 400     2 900     2 100 peak  7412 weight  0 10000E+01 volume  0 55913E+02 ppm1      4 164 ppm2      1 645
ASSI { 7422}
  (( segid "BrD " and resid 46    and name HA  ))
  (  segid "BrD " and resid 43    and name HB% )
     3 600     3.200     1 900 peak  7422 weight  0 10000E+01 volume  0 39252E+02 ppm1      4 164 ppm2      1 718
ASSI { 7442}
  (( segid "BrD " and resid 68    and name HA  ))
  (  segid "BrD " and resid 63    and name HD1%)
     3 700     3 400     1 800 peak  7442 weight  0 10000E+01 volume  0 32100E+02 ppm1      5 146 ppm2      1 653
ASSI { 7462}
  (( segid "BrD " and resid 68    and name HB2 ))
  (  segid "BrD " and resid 18    and name HD1%)
     3 100     2 400     2 400 peak  7462 weight  0 10000E+01 volume  0 95501E+02 ppm1      3 522 ppm2      1 083
ASSI { 7472}
  (( segid "BrD " and resid 68    and name HB1 ))
  (  segid "BrD " and resid 18    and name HD1%)
     3 100     2 400     2 400 peak  7472 weight  0 10000E+01 volume  0 86786E+02 ppm1      3 669 ppm2      1 084
ASSI { 8082}
  (( segid "BrD " and resid 98    and name HA  ))
  (( segid "BrD " and resid 30    and name HB2 ))
     2 900     2 100     2 100 peak  8082 weight  0 10000E+01 volume  0 14301E+03 ppm1      4 802 ppm2      4 530
ASSI { 8132}
  (  segid "BrD " and resid 63    and name HD1%)
  (( segid "BrD " and resid 15    and name HA  ))
     2 800     2 000     2 000 peak  8132 weight  0 10000E+01 volume  0 17717E+03 ppm1      1 646 ppm2      4 624
ASSI { 8252}
  (( segid "BrD " and resid 109   and name HG1 ))
  (( segid "BrD " and resid 109   and name HD1 ))
     2 700     1.800     1.800 peak  8252 weight  0 10000E+01 volume  0 20695E+03 ppm1      1 401 ppm2      1 989
ASSI { 8282}
  (( segid "BrD " and resid 18    and name HA  ))
  (( segid "BrD " and resid 21    and name HG12))
     3.300     2 700     2 200 peak  8282 weight  0 10000E+01 volume  0 61204E+02 ppm1      3 866 ppm2      1 640
ASSI { 8362}
  (( segid "BrD " and resid 18    and name HG  ))
  (  segid "BrD " and resid 14    and name HD2%)
     3 100     2.400     2.400 peak  8362 weight  0 10000E+01 volume  0.89516E+02 ppm1      2 290 ppm2      1 418
OR { 8362}
  (( segid "BrD " and resid 18    and name HG  ))
  (  segid "BrD " and resid 14    and name HD1%)
ASSI { 8422}
  (  segid "BrD " and resid 18    and name HD1%)
  (( segid "BrD " and resid 14    and name HG  ))
     2 700     1.800     1 800 peak  8422 weight  0 10000E+01 volume  0 21908E+03 ppm1      1 058 ppm2      2 070
ASSI { 8432}
  (  segid "BrD " and resid 18    and name HD1%)
  (( segid "BrD " and resid 15    and name HA  ))
     2 700     1.800     1.800 peak  8432 weight  0 10000E+01 volume  0 20923E+03 ppm1      1 057 ppm2      4 626
ASSI { 8512}
  (  segid "BrD " and resid 22    and name HD2%)
  (  segid "BrD " and resid 78    and name HD2%)
     3 300     2 700     2 200 peak  8512 weight  0 10000E+01 volume  0 62220E+02 ppm1      1 599 ppm2      0 677
ASSI { 8522}
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   ( segid "BrD " and resid 22   and name HD2%)
   ( segid "BrD " and resid 59   and name HE% )
     2 900     2 100     2 100 peak  8522 weight  0 10000E+01 volume  0 12491E+03 ppm1     1 599 ppm2     1 871
ASSI { 8532}
   ( segid "BrD " and resid 22   and name HD1%)
   (( segid "BrD " and resid 60   and name HA  ))
     2.600     1 700     1.700 peak  8532 weight  0 10000E+01 volume  0 23265E+03 ppm1     1 645 ppm2     4 809
ASSI { 8582}
   (( segid "BrD " and resid 22   and name HB2 ))
   ( segid "BrD " and resid 63   and name HD2%)
     2 600     1 700     1 700 peak  8582 weight  0 10000E+01 volume  0 24738E+03 ppm1     2 286 ppm2     1 494
ASSI { 8612}
   (( segid "BrD " and resid 56   and name HB1 ))
   (( segid "BrD " and resid 35   and name HA  ))
     2 800     2 000     2 000 peak  8612 weight  0 10000E+01 volume  0 17130E+03 ppm1     2 685 ppm2     4 900
ASSI { 8632}
   ( segid "BrD " and resid 56   and name HD1%)
   ( segid "BrD " and resid 81   and name HG2%)
     3 800     3 600     1.700 peak  8632 weight  0 10000E+01 volume  0 24706E+02 ppm1     1 547 ppm2     0 758
ASSI { 8642}
   (( segid "BrD " and resid 116  and name HG12))
   (( segid "BrD " and resid 116  and name HG11))
     2 000     1 000     1 000 peak  8642 weight  0 10000E+01 volume  0.13013E+04 ppm1     1 548 ppm2     1 921
ASSI { 8702}
   ( segid "BrD " and resid 56   and name HD2%)
   ( segid "BrD " and resid 81   and name HG1%)
     2 400     1.400     1 400 peak  8702 weight  0 10000E+01 volume  0 46717E+03 ppm1     1 254 ppm2     1 080
ASSI { 8832}
   ( segid "BrD " and resid 78   and name HD1%)
   (( segid "BrD " and resid 18   and name HB2 ))
     4 100     4 100     1 400 peak  8832 weight  0 10000E+01 volume  0 15698E+02 ppm1     0 761 ppm2     0 924
ASSI { 8882}
   ( segid "BrD " and resid 78   and name HD2%)
   ( segid "BrD " and resid 18   and name HD2%)
     3.000     2 200     2 200 peak  8882 weight  0 10000E+01 volume  0 10893E+03 ppm1     0 662 ppm2     0 427
ASSI { 8942}
   (( segid "BrD " and resid 102  and name HA  ))
   ( segid "BrD " and resid 101  and name HG2%)
     3 100     2 400     2 400 peak  8942 weight  0 10000E+01 volume  0 83720E+02 ppm1     4 263 ppm2     1 612
ASSI { 9102}
   (( segid "BrD " and resid 21   and name HG12))
   ( segid "BrD " and resid 102  and name HD2%)
     3.700     3.400     1 800 peak  9102 weight  0 10000E+01 volume  0 31128E+02 ppm1     1 648 ppm2     1 320
OR { 9102}
   (( segid "BrD " and resid 21   and name HG12))
   ( segid "BrD " and resid 102  and name HD1%)
ASSI { 9122}
   ( segid "BrD " and resid 21   and name HG2%)
   ( segid "BrD " and resid 110  and name HD1%)
     2 900     2 100     2.100 peak  9122 weight  0 10000E+01 volume  0 12723E+03 ppm1     1 600 ppm2     1 143
ASSI { 9132}
   ( segid "BrD " and resid 21   and name HG2%)
   ( segid "BrD " and resid 78   and name HD2%)
     3 400     2 900     2 100 peak  9132 weight  0 10000E+01 volume  0 50284E+02 ppm1     1 596 ppm2     0 670
ASSI { 9172}
   ( segid "BrD " and resid 21   and name HD1%)
   ( segid "BrD " and resid 17   and name HG2%)
     2 500     1 600     1 600 peak  9172 weight  0 10000E+01 volume  0.33280E+03 ppm1     1 205 ppm2     1.748
ASSI { 9402}
   ( segid "BrD " and resid 21   and name HG2%)
   (( segid "BrD " and resid 106  and name HA  ))
     2 600     1 700     1 700 peak  9402 weight  0 10000E+01 volume  0 25016E+03 ppm1     1 597 ppm2     4 536
ASSI { 9412}
   ( segid "BrD " and resid 101  and name HG2%)
   (( segid "BrD " and resid 30   and name HB1 ))
     2 800     2 000     2 000 peak  9412 weight  0 10000E+01 volume  0 17182E+03 ppm1     1 598 ppm2     4 928
ASSI { 9462}
   (( segid "BrD " and resid 110  and name HB  ))
   (( segid "BrD " and resid 115  and name HB1 ))
     3.000     2 200     2 200 peak  9462 weight  0 10000E+01 volume  0 11040E+03 ppm1     2 338 ppm2     2 182
ASSI { 9502}
   ( segid "BrD " and resid 110  and name HG2%)
   (( segid "BrD " and resid 115  and name HB1 ))
     2 500     1 600     1 600 peak  9502 weight  0 10000E+01 volume  0 34762E+03 ppm1     1 252 ppm2     2.182
ASSI { 9512}
   ( segid "BrD " and resid 110  and name HG2%)
   (( segid "BrD " and resid 116  and name HG12))
     2 500     1 600     1 600 peak  9512 weight  0 10000E+01 volume  0 33973E+03 ppm1     1.253 ppm2     1 586
ASSI { 9572}
   ( segid "BrD " and resid 110  and name HD1%)
   ( segid "BrD " and resid 78   and name HD1%)
     3 800     3 600     1 700 peak  9572 weight  0 10000E+01 volume  0 27664E+02 ppm1     1 154 ppm2     0 750
ASSI { 9602}
   ( segid "BrD " and resid 110  and name HD1%)
   ( segid "BrD " and resid 78   and name HD2%)
     3 400     2 900     2.100 peak  9602 weight  0 10000E+01 volume  0 49420E+02 ppm1     1 154 ppm2     0.676
ASSI { 9622}
   ( segid "BrD " and resid 116  and name HG2%)
   ( segid "BrD " and resid 110  and name HG2%)
     2 800     2 000     2 000 peak  9622 weight  0.10000E+01 volume  0 18357E+03 ppm1     1.401 ppm2     1 271
ASSI { 9632}
   ( segid "BrD " and resid 116  and name HD1%)
   ( segid "BrD " and resid 110  and name HD1%)
     2 100     1 100     1 100 peak  9632 weight  0 10000E+01 volume  0 89032E+03 ppm1     1 399 ppm2     1 152
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ASSI { 9992}
   (( segid "BrD " and resid 54   and name HB2 ))
   (( segid "BrD " and resid 59   and name HB2 ))
     2.700     1.800     1 800 peak  9992 weight  0 10000E+01 volume  0 19570E+03 ppm1     1 947 ppm2     2 490
ASSI {10032}
   (( segid "BrD " and resid 54   and name HA  ))
   (( segid "BrD " and resid 59   and name HB2 ))
     3 000     2.200     2 200 peak 10032 weight  0 10000E+01 volume  0 99741E+02 ppm1     5 541 ppm2     2 481
ASSI {10142}
   (( segid "BrD " and resid 70   and name HB2 ))
   (( segid "BrD " and resid 73   and name HB1 ))
     4 100     4 100     1 400 peak 10142 weight  0.10000E+01 volume  0 17585E+02 ppm1     4 360 ppm2     2 597
ASSI {10172}
   (( segid "BrD " and resid 52   and name HB2 ))
   (( segid "BrD " and resid 80   and name HG1 ))
     4 200     4.200     1 300 peak 10172 weight  0 10000E+01 volume  0 15368E+02 ppm1     3 522 ppm2     2 345
ASSI {10512}
   (( segid "BrD " and resid 61   and name HG1 ))
   (( segid "BrD " and resid 60   and name HB2 ))
     2.700     1 800     1 800 peak 10512 weight  0 10000E+01 volume  0 19616E+03 ppm1     2.980 ppm2     4 588
ASSI {10832}
   (( segid "BrD " and resid 30   and name HB1 ))
   ( segid "BrD " and resid 102  and name HD1%)
     3 600     3 200     1 900 peak 10832 weight  0 10000E+01 volume  0 34957E+02 ppm1     4 907 ppm2     1 329
ASSI {10842}
   (( segid "BrD " and resid 30   and name HB2 ))
   ( segid "BrD " and resid 102  and name HD1%)
     3.200     2 600     2 300 peak 10842 weight  0 10000E+01 volume  0 80809E+02 ppm1     4 510 ppm2     1 320
ASSI {10912}
   (( segid "BrD " and resid 93   and name HB1 ))
   (( segid "BrD " and resid 91   and name HG1 ))
     3 700     3 400     1 800 peak 10912 weight  0 10000E+01 volume  0 32594E+02 ppm1     5 000 ppm2     2.798
ASSI {10922}
   (( segid "BrD " and resid 93   and name HB2 ))
   (( segid "BrD " and resid 91   and name HG1 ))
     3 700     3 400     1 800 peak 10922 weight  0 10000E+01 volume  0 31695E+02 ppm1     4 755 ppm2     2 799
ASSI {10962}
   (( segid "BrD " and resid 44   and name HA  ))
   (( segid "BrD " and resid 41   and name HA  ))
     4 600     4.600     0 900 peak 10962 weight  0 10000E+01 volume  0 78869E+01 ppm1     5 099 ppm2     4.654
ASSI {11342}
   (( segid "BrD " and resid 19   and name HG1 ))
   ( segid "BrD " and resid 63   and name HD2%)
     3 100     2 400     2 400 peak 11342 weight  0 10000E+01 volume  0 91996E+02 ppm1     1 889 ppm2     1 493
ASSI {11372}
   (( segid "BrD " and resid 26   and name HA  ))
   ( segid "BrD " and resid 31   and name HB% )
     2 200     1 200     1 200 peak 11372 weight  0 10000E+01 volume  0 67300E+03 ppm1     4 509 ppm2     2 311
ASSI {11382}
   (( segid "BrD " and resid 26   and name HA  ))
   ( segid "BrD " and resid 35   and name HE% )
     2 800     2 000     2 000 peak 11382 weight  0 10000E+01 volume  0 18352E+03 ppm1     4 509 ppm2     2 783
ASSI {11502}
   (( segid "BrD " and resid 86   and name HE1 ))
   (( segid "BrD " and resid 83   and name HA  ))
     2 900     2 100     2 100 peak 11502 weight  0 10000E+01 volume  0 14787E+03 ppm1     3 080 ppm2     4 460
ASSI {11572}
   (( segid "BrD " and resid 109  and name HB1 ))
   ( segid "BrD " and resid 21   and name HG2%)
     3 500     3 100     2 000 peak 11572 weight  0 10000E+01 volume  0 46116E+02 ppm1     2 334 ppm2     1.587
ASSI {11642}
   (( segid "BrD " and resid 6    and name HB2 ))
   (( segid "BrD " and resid 7    and name HG1 ))
     3 100     2 400     2 400 peak 11642 weight  0 10000E+01 volume  0 90515E+02 ppm1     2 291 ppm2     2 876
ASSI {11752}
   (( segid "BrD " and resid 55   and name HB1 ))
   (( segid "BrD " and resid 37   and name HA  ))
     2 800     2 000     2 000 peak 11752 weight  0 10000E+01 volume  0 16032E+03 ppm1     2 979 ppm2     4 860
ASSI {11832}
   (( segid "BrD " and resid 91   and name HA  ))
   (( segid "BrD " and resid 92   and name HB2 ))
     3 500     3 100     2 000 peak 11832 weight  0 10000E+01 volume  0 43713E+02 ppm1     5 347 ppm2     2 571
ASSI {12292}
   ( segid "BrD " and resid 81   and name HG2%)
   (( segid "BrD " and resid 56   and name HG  ))
     3 300     2 700     2 200 peak 12292 weight  0 10000E+01 volume  0 58134E+02 ppm1     0 761 ppm2     2 323
ASSI {12502}
   (( segid "BrD " and resid 54   and name HG1 ))
   (( segid "BrD " and resid 59   and name HB2 ))
     4 000     4.000     1 500 peak 12502 weight  0 10000E+01 volume  0 18992E+02 ppm1     3 288 ppm2     2 467
ASSI {12632}
   ( segid "BrD " and resid 59   and name HE% )
   (( segid "BrD " and resid 77   and name HB1 ))
     2 500     1.600     1 600 peak 12632 weight  0 10000E+01 volume  0 30644E+03 ppm1     1 848 ppm2     3.321
ASSI {12732}
   (( segid "BrD " and resid 71   and name HA  ))
   ( segid "BrD " and resid 18   and name HD1%)
     3.700     3.400     1 800 peak 12732 weight  0 10000E+01 volume  0 29522E+02 ppm1     4 608 ppm2     1 084
ASSI {12752}
   (( segid "BrD " and resid 71   and name HA  ))
   ( segid "BrD " and resid 18   and name HD2%)
     3 300     2.700     2 200 peak 12752 weight  0 10000E+01 volume  0 66213E+02 ppm1     4 607 ppm2     0 409
ASSI {12872}
   (( segid "BrD " and resid 62   and name HD1 ))
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  (( segid "BrD " and resid 59   and name HB2 ))
     3.500      3.100      2.000 peak 12872 weight  0.10000E+01 volume  0.44554E+02 ppm1       3.177 ppm2       2.484
ASSI {13092}
  (( segid "BrD " and resid 54   and name HG1 ))
   ( segid "BrD " and resid 81   and name HG1%)
     3 400      2 900      2.100 peak 13092 weight  0 10000E+01 volume  0 51686E+02 ppm1       3 288 ppm2       1 075
ASSI {13112}
  (( segid "BrD " and resid 73   and name HB2 ))
  (( segid "BrD " and resid 68   and name HA  ))
     3 000      2.200      2.200 peak 13112 weight  0 10000E+01 volume  0 10760E+03 ppm1       2 486 ppm2       5 142
ASSI {13122}
  (( segid "BrD " and resid 73   and name HB1 ))
  (( segid "BrD " and resid 68   and name HA  ))
     2 900      2 100      2 100 peak 13122 weight  0 10000E+01 volume  0 13268E+03 ppm1       2 583 ppm2       5 141
ASSI {13232}
  (( segid "BrD " and resid 46   and name HB1 ))
   ( segid "BrD " and resid 38   and name HG2%)
     3 500      3 100      2 000 peak 13232 weight  0 10000E+01 volume  0 45934E+02 ppm1       3 275 ppm2       0 790
ASSI {13282}
  (( segid "BrD " and resid 56   and name HA  ))
   ( segid "BrD " and resid 22   and name HD2%)
     3 100      2.400      2 400 peak 13282 weight  0 10000E+01 volume  0 86018E+02 ppm1       4 607 ppm2       1.637
OR {13282}
  (( segid "BrD " and resid 56   and name HA  ))
   ( segid "BrD " and resid 22   and name HD1%)
ASSI {13312}
  (( segid "BrD " and resid 116  and name HG12))
   ( segid "BrD " and resid 110  and name HD1%)
     2 700      1.800      1 800 peak 13312 weight  0 10000E+01 volume  0 18778E+03 ppm1       1 548 ppm2       1 145
ASSI {13332}
   ( segid "BrD " and resid 22   and name HD1%)
  (( segid "BrD " and resid 63   and name HB2 ))
     2 500      1 600      1 600 peak 13332 weight  0 10000E+01 volume  0 34390E+03 ppm1       1 648 ppm2       2 516
ASSI {13412}
   ( segid "BrD " and resid 25   and name HG1%)
   ( segid "BrD " and resid 56   and name HD2%)
     2 900      2 100      2 100 peak 13412 weight  0 10000E+01 volume  0 12726E+03 ppm1       1 795 ppm2       1 252
ASSI {13572}
  (( segid "BrD " and resid 49   and name HB  ))
  (( segid "BrD " and resid 50   and name HG11))
     5 500      5 500      0 000 peak 13572 weight  0 10000E+01 volume  0 27123E-01 ppm1       2 634 ppm2       1 417
ASSI {13582}
  (( segid "BrD " and resid 49   and name HB  ))
   ( segid "BrD " and resid 50   and name HD1%)
     4 000      4 000      1 500 peak 13582 weight  0 10000E+01 volume  0 18896E+02 ppm1       2 634 ppm2       1 148
ASSI {13682}
   ( segid "BrD " and resid 54   and name HE% )
  (( segid "BrD " and resid 57   and name HG1 ))
     3.600      3 200      1 900 peak 13682 weight  0.10000E+01 volume  0 37432E+02 ppm1       2 537 ppm2       2.101
ASSI {13732}
  (( segid "BrD " and resid 63   and name HA  ))
  (( segid "BrD " and resid 68   and name HB1 ))
     3 500      3 100      2 000 peak 13732 weight  0 10000E+01 volume  0 44471E+02 ppm1       5 296 ppm2       3.662
ASSI {13752}
   ( segid "BrD " and resid 63   and name HD2%)
  (( segid "BrD " and resid 19   and name HB2 ))
     2 700      1 800      1 800 peak 13752 weight  0 10000E+01 volume  0 20264E+03 ppm1       1 498 ppm2       1 996
ASSI {13772}
  (( segid "BrD " and resid 64   and name HA  ))
   ( segid "BrD " and resid 63   and name HD2%)
     4.000      4.000      1 500 peak 13772 weight  0 10000E+01 volume  0 18294E+02 ppm1       4 951 ppm2       1 488
ASSI {13792}
   ( segid "BrD " and resid 49   and name HG1%)
   ( segid "BrD " and resid 50   and name HG2%)
     3.800      3 600      1 700 peak 13792 weight  0 10000E+01 volume  0 26015E+02 ppm1       1 646 ppm2       1.009
ASSI {13812}
  (( segid "BrD " and resid 76   and name HA  ))
  (( segid "BrD " and resid 80   and name HB2 ))
     4.200      4 200      1 300 peak 13812 weight  0 10000E+01 volume  0 14558E+02 ppm1       4 656 ppm2       2.508
ASSI {13832}
  (( segid "BrD " and resid 56   and name HB1 ))
  (( segid "BrD " and resid 34   and name HB2 ))
     3 100      2 400      2 400 peak 13832 weight  0 10000E+01 volume  0 92421E+02 ppm1       2 685 ppm2       3 159
ASSI {13842}
  (( segid "BrD " and resid 67   and name HB2 ))
  (( segid "BrD " and resid 62   and name HA  ))
     3 400      2.900      2 100 peak 13842 weight  0 10000E+01 volume  0 56015E+02 ppm1       2 636 ppm2       4 483
ASSI {13862}
   ( segid "BrD " and resid 69   and name HG2%)
   ( segid "BrD " and resid 18   and name HD1%)
     3 600      3 200      1 900 peak 13862 weight  0 10000E+01 volume  0.35688E+02 ppm1       1 425 ppm2       1 030
ASSI {13872}
   ( segid "BrD " and resid 69   and name HG2%)
  (( segid "BrD " and resid 18   and name HB2 ))
     5 500      5 500      0 000 peak 13872 weight  0.10000E+01 volume  0.14355E+01 ppm1       1 425 ppm2       0 880
ASSI {13892}
  (( segid "BrD " and resid 12   and name HA  ))
   ( segid "BrD " and resid 14   and name HD2%)
     3 000      2 200      2 200 peak 13892 weight  0.10000E+01 volume  0 11539E+03 ppm1       5 298 ppm2       1 382
OR {13892}
  (( segid "BrD " and resid 12   and name HA  ))
   ( segid "BrD " and resid 14   and name HD1%)
ASSI {13982}
  (( segid "BrD " and resid 74   and name HA  ))
  (( segid "BrD " and resid 68   and name HB2 ))
     3.600      3.200      1.900 peak 13982 weight  0.10000E+01 volume  0.36366E+02 ppm1       4 360 ppm2       3 499
ASSI {14032}
   ( segid "BrD " and resid 76   and name HB% )
  (( segid "BrD " and resid 80   and name HG1 ))
     2.800      2 000      2 000 peak 14032 weight  0 10000E+01 volume  0.17944E+03 ppm1       2 091 ppm2       2 344
ASSI {14052}
   ( segid "BrD " and resid 14   and name HD1%)
  (( segid "BrD " and resid 70   and name HA  ))
     2 700      1 800      1 800 peak 14052 weight  0 10000E+01 volume  0.21486E+03 ppm1       1.402 ppm2       5 362
ASSI {14112}
  (( segid "BrD " and resid 14   and name HA  ))
   ( segid "BrD " and resid 113  and name HB% )
     3 100      2 400      2 400 peak 14112 weight  0 10000E+01 volume  0 82177E+02 ppm1       4 655 ppm2       1 987
ASSI {14212}
  (( segid "BrD " and resid 98   and name HB2 ))
  (( segid "BrD " and resid 30   and name HB1 ))
     3 700      3 400      1 800 peak 14212 weight  0 10000E+01 volume  0 32251E+02 ppm1       3 667 ppm2       4 933
ASSI {14222}
  (( segid "BrD " and resid 99   and name HA  ))
  (( segid "BrD " and resid 102  and name HG  ))
     3 400      2 900      2 100 peak 14222 weight  0 10000E+01 volume  0 54061E+02 ppm1       4.459 ppm2       2 136
ASSI {14242}
  (( segid "BrD " and resid 99   and name HA  ))
  (( segid "BrD " and resid 82   and name HB2 ))
     3.000      2.200      2 200 peak 14242 weight  0 10000E+01 volume  0.10335E+03 ppm1       4 457 ppm2       3 581
ASSI {14262}
  (( segid "BrD " and resid 31   and name HA  ))
  (( segid "BrD " and resid 33   and name HD2 ))
     3 300      2 700      2 200 peak 14262 weight  0 10000E+01 volume  0 61370E+02 ppm1       5 000 ppm2       2 218
ASSI {14272}
   ( segid "BrD " and resid 31   and name HB% )
  (( segid "BrD " and resid 25   and name HA  ))
     3 000      2 200      2 200 peak 14272 weight  0 10000E+01 volume  0 10586E+03 ppm1       2 289 ppm2       4 437
ASSI {14292}
  (( segid "BrD " and resid 110  and name HB  ))
   ( segid "BrD " and resid 115  and name HD1%)
     5 500      5 500      0 000 peak 14292 weight  0 10000E+01 volume  0 49515E+00 ppm1       2 338 ppm2       1 318
ASSI {14302}
   ( segid "BrD " and resid 63   and name HD2%)
  (( segid "BrD " and resid 22   and name HB1 ))
     2 500      1 600      1 600 peak 14302 weight  0 10000E+01 volume  0 30120E+03 ppm1       1 498 ppm2       2 695
ASSI {14332}
  (( segid "BrD " and resid 103  and name HA  ))
  (( segid "BrD " and resid 102  and name HB2 ))
     3 500      3 100      2 000 peak 14332 weight  0 10000E+01 volume  0 41084E+02 ppm1       3 769 ppm2       1 830
ASSI {14352}
  (( segid "BrD " and resid 106  and name HA  ))
  (( segid "BrD " and resid 109  and name HG1 ))
     4 000      4 000      1 500 peak 14352 weight  0 10000E+01 volume  0 19913E+02 ppm1       4 555 ppm2       1 435
ASSI {14382}
  (( segid "BrD " and resid 15   and name HA  ))
  (( segid "BrD " and resid 14   and name HG  ))
     3 800      3 600      1 700 peak 14382 weight  0 10000E+01 volume  0 25435E+02 ppm1       4 606 ppm2       2 042
ASSI {14442}
  (( segid "BrD " and resid 110  and name HA  ))
  (( segid "BrD " and resid 115  and name HB1 ))
     2 800      2 000      2 000 peak 14442 weight  0 10000E+01 volume  0 18018E+03 ppm1       4 411 ppm2       2 181
OR {14442}
  (( segid "BrD " and resid 110  and name HA  ))
  (( segid "BrD " and resid 115  and name HG  ))
ASSI {14452}
   ( segid "BrD " and resid 110  and name HG2%)
   ( segid "BrD " and resid 115  and name HD1%)
     2 600      1 700      1 700 peak 14452 weight  0 10000E+01 volume  0 23487E+03 ppm1       1.254 ppm2       1 330
ASSI {14512}
  (( segid "BrD " and resid 111  and name HG1 ))
   ( segid "BrD " and resid 110  and name HG2%)
     3 600      3 200      1 900 peak 14512 weight  0 10000E+01 volume  0 36391E+02 ppm1       1 989 ppm2       1.278
ASSI {14652}
  (( segid "BrD " and resid 18   and name HA  ))
  (( segid "BrD " and resid 21   and name HG11))
     3 700      3 400      1 800 peak 14652 weight  0 10000E+01 volume  0 30202E+02 ppm1       3 866 ppm2       2 351
ASSI {14672}
   ( segid "BrD " and resid 18   and name HD1%)
  (( segid "BrD " and resid 63   and name HG  ))
     3 100      2 400      2 400 peak 14672 weight  0 10000E+01 volume  0 91159E+02 ppm1       1 057 ppm2       2.467
ASSI {14702}
   ( segid "BrD " and resid 21   and name HD1%)
   ( segid "BrD " and resid 63   and name HD2%)
     2 300      2 300      2 200 peak 14702 weight  0 10000E+01 volume  0.60922E+03 ppm1       1 205 ppm2       1 458
ASSI {14752}
   ( segid "BrD " and resid 54   and name HE% )
   ( segid "BrD " and resid 81   and name HG1%)
     3 700      3 400      1 800 peak 14752 weight  0 10000E+01 volume  0 28669E+02 ppm1       2.535 ppm2       1.075
ASSI {14762}
  (( segid "BrD " and resid 51   and name HA  ))
  (( segid "BrD " and resid 53   and name HD1 ))
     5.500      5 500      0.000 peak 14762 weight  0 10000E+01 volume  0 89215E-01 ppm1       4 460 ppm2       4 222
ASSI {14782}
  (( segid "BrD " and resid 36   and name HA  ))
  (( segid "BrD " and resid 57   and name HB1 ))
     2 300      1 300      1 300 peak 14782 weight  0 10000E+01 volume  0 60436E+03 ppm1       5 446 ppm2       2 956
ASSI {15012}
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  (( segid "BrD " and resid 46   and name HB1 ))
  (  segid "BrD " and resid 38   and name HG1%)
     4 000     4.000     1 500 peak 15012 weight  0 10000E+01 volume  0 20055E+02 ppm1     3 275 ppm2     1 075
ASSI {15032}
  (( segid "BrD " and resid 46   and name HB1 ))
  (  segid "BrD " and resid 47   and name HD% )
     4.500     4 500     1 000 peak 15032 weight  0 10000E+01 volume  0.96365E+01 ppm1     3 276 ppm2     7 934
ASSI {15042}
  (( segid "BrD " and resid 46   and name HB2 ))
  (  segid "BrD " and resid 47   and name HD% )
     3 200     2 600     2.300 peak 15042 weight  0 10000E+01 volume  0 71990E+02 ppm1     3 077 ppm2     7 933
ASSI {15052}
  (( segid "BrD " and resid 46   and name HA  ))
  (  segid "BrD " and resid 49   and name HG2%)
     3 600     3 200     1 900 peak 15052 weight  0 10000E+01 volume  0.38868E+02 ppm1     4 165 ppm2     1 571
ASSI {15092}
  (( segid "BrD " and resid 28   and name HB2 ))
  (  segid "BrD " and resid 31   and name HB% )
     2 800     2 000     2 000 peak 15092 weight  0.10000E+01 volume  0 15966E+03 ppm1     3 374 ppm2     2 312
ASSI {15182}
  (( segid "BrD " and resid 67   and name HB1 ))
  (( segid "BrD " and resid 62   and name HB2 ))
     4 000     4 000     1 500 peak 15182 weight  0 10000E+01 volume  0 19603E+02 ppm1     3 572 ppm2     1 693
ASSI {15192}
  (( segid "BrD " and resid 67   and name HB1 ))
  (( segid "BrD " and resid 62   and name HG2 ))
     4 400     4.400     1 100 peak 15192 weight  0 10000E+01 volume  0 11033E+02 ppm1     3 572 ppm2     1 474
ASSI {15402}
  (( segid "BrD " and resid 82   and name HB2 ))
  (  segid "BrD " and resid 99   and name HB% )
     3 000     2 200     2 200 peak 15402 weight  0 10000E+01 volume  0.10551E+03 ppm1     3 572 ppm2     2 206
ASSI {15412}
  (( segid "BrD " and resid 82   and name HB1 ))
  (  segid "BrD " and resid 99   and name HB% )
     2 900     2 100     2 100 peak 15412 weight  0 10000E+01 volume  0 12753E+03 ppm1     3 672 ppm2     2 206
ASSI {15552}
  (( segid "BrD " and resid 82   and name HB2 ))
  (( segid "BrD " and resid 103  and name HB2 ))
     3 700     3 400     1 800 peak 15552 weight  0 10000E+01 volume  0 31328E+02 ppm1     3 573 ppm2     1 897
ASSI {15592}
  (( segid "BrD " and resid 107  and name HB1 ))
  (( segid "BrD " and resid 103  and name HG3 ))
     3.100     2 400     2 400 peak 15592 weight  0 10000E+01 volume  0 86957E+02 ppm1     3 670 ppm2     2 540
ASSI {15712}
  (( segid "BrD " and resid 107  and name HB1 ))
  (  segid "BrD " and resid 107  and name HD% )
     2.200     1 200     1 200 peak 15712 weight  0 10000E+01 volume  0 63746E+03 ppm1     3 673 ppm2     7 827
ASSI {15812}
  (( segid "BrD " and resid 15   and name HA  ))
  (( segid "BrD " and resid 18   and name HA  ))
     3 300     2 700     2 200 peak 15812 weight  0 10000E+01 volume  0 67333E+02 ppm1     4 606 ppm2     3 900
ASSI {15882}
  (( segid "BrD " and resid 15   and name HB1 ))
  (  segid "BrD " and resid 63   and name HD1%)
     4 000     4 000     1 500 peak 15882 weight  0 10000E+01 volume  0 19033E+02 ppm1     3 815 ppm2     1 652
ASSI {15932}
  (( segid "BrD " and resid 82   and name HB1 ))
  (( segid "BrD " and resid 107  and name HZ  ))
     2 600     1 700     1 700 peak 15932 weight  0 10000E+01 volume  0 26167E+03 ppm1     3 670 ppm2     8.022
ASSI {16052}
  (( segid "BrD " and resid 68   and name HA  ))
  (( segid "BrD " and resid 73   and name HG  ))
     4 000     4 000     1 500 peak 16052 weight  0 10000E+01 volume  0 20921E+02 ppm1     5 148 ppm2     2.367
ASSI {16062}
  (( segid "BrD " and resid 68   and name HB2 ))
  (  segid "BrD " and resid 74   and name HD% )
     3 600     3 200     1 900 peak 16062 weight  0.10000E+01 volume  0 38285E+02 ppm1     3 522 ppm2     6 998
ASSI {16112}
  (( segid "BrD " and resid 68   and name HB1 ))
  (( segid "BrD " and resid 62   and name HD1 ))
     4 500     4 500     1 000 peak 16112 weight  0 10000E+01 volume  0 90000E+01 ppm1     3 669 ppm2     3 148
ASSI {16122}
  (( segid "BrD " and resid 68   and name HB2 ))
  (( segid "BrD " and resid 62   and name HD1 ))
     3.500     3 100     2 000 peak 16122 weight  0 10000E+01 volume  0 43825E+02 ppm1     3 522 ppm2     3 149
ASSI {16132}
  (( segid "BrD " and resid 68   and name HB1 ))
  (( segid "BrD " and resid 63   and name HB1 ))
     3 600     3 200     1.900 peak 16132 weight  0 10000E+01 volume  0.35724E+02 ppm1     3 669 ppm2     2 883
ASSI {16152}
  (( segid "BrD " and resid 68   and name HB2 ))
  (( segid "BrD " and resid 63   and name HB1 ))
     3 500     3 100     2 000 peak 16152 weight  0 10000E+01 volume  0.44106E+02 ppm1     3 522 ppm2     2 884
ASSI {16162}
  (( segid "BrD " and resid 68   and name HB2 ))
  (( segid "BrD " and resid 62   and name HB1 ))
     4 100     4.100     1 400 peak 16162 weight  0 10000E+01 volume  0 16622E+02 ppm1     3 522 ppm2     2 605
ASSI {16212}
  (( segid "BrD " and resid 88   and name HA  ))
  (  segid "BrD " and resid 49   and name HG2%)
     3 200     2 600     2 300 peak 16212 weight  0 10000E+01 volume  0.71276E+02 ppm1     4 999 ppm2     1 571
ASSI {16312}
  (( segid "BrD " and resid 88   and name HB1 ))
  (  segid "BrD " and resid 95   and name HD% )
     3.500     3.100     2.000 peak 16312 weight  0.10000E+01 volume  0.47079E+02 ppm1     3.524 ppm2     7.496
ASSI {16382}
  (( segid "BrD " and resid 19   and name HE1 ))
  (  segid "BrD " and resid 63   and name HD2%)
     3 500     3.100     2 000 peak 16382 weight  0 10000E+01 volume  0 45471E+02 ppm1     3 522 ppm2     1 495
ASSI {16422}
  (( segid "BrD " and resid 66   and name HD2 ))
  (  segid "BrD " and resid 69   and name HG1%)
     4.900     4 900     0 600 peak 16422 weight  0 10000E+01 volume  0 59473E+01 ppm1     3 621 ppm2     1 562
ASSI {16432}
  (( segid "BrD " and resid 66   and name HD2 ))
  (  segid "BrD " and resid 63   and name HD1%)
     4 700     4 700     0.800 peak 16432 weight  0 10000E+01 volume  0.72449E+01 ppm1     3 620 ppm2     1 645
ASSI {16492}
  (( segid "BrD " and resid 96   and name HA  ))
  (( segid "BrD " and resid 86   and name HA  ))
     2 200     1 200     1 200 peak 16492 weight  0.10000E+01 volume  0 78759E+03 ppm1     4 409 ppm2     4 802
ASSI {16502}
  (( segid "BrD " and resid 96   and name HA  ))
  (( segid "BrD " and resid 86   and name HG2 ))
     4 100     4 100     1 400 peak 16502 weight  0.10000E+01 volume  0 17647E+02 ppm1     4 409 ppm2     0 758
ASSI {16612}
  (( segid "BrD " and resid 96   and name HB2 ))
  (  segid "BrD " and resid 96   and name HE% )
     3 400     2 900     2 100 peak 16612 weight  0 10000E+01 volume  0 47985E+02 ppm1     3 134 ppm2     7 632
ASSI {16662}
  (( segid "BrD " and resid 96   and name HB1 ))
  (  segid "BrD " and resid 99   and name HB% )
     4 200     4.200     1.300 peak 16662 weight  0 10000E+01 volume  0 14266E+02 ppm1     4 008 ppm2     2 227
ASSI {16672}
  (( segid "BrD " and resid 96   and name HB2 ))
  (  segid "BrD " and resid 99   and name HB% )
     4 200     4 200     1 300 peak 16672 weight  0 10000E+01 volume  0 13986E+02 ppm1     3 125 ppm2     2 209
ASSI {16682}
  (( segid "BrD " and resid 52   and name HA  ))
  (( segid "BrD " and resid 53   and name HG1 ))
     4 300     4 300     1 200 peak 16682 weight  0 10000E+01 volume  0 11894E+02 ppm1     5 589 ppm2     2.819
OR {16682}
  (( segid "BrD " and resid 52   and name HA  ))
  (( segid "BrD " and resid 53   and name HB1 ))
ASSI {16792}
  (( segid "BrD " and resid 95   and name HB2 ))
  (( segid "BrD " and resid 85   and name HA  ))
     2 700     1 800     1 800 peak 16792 weight  0 10000E+01 volume  0 22870E+03 ppm1     3 375 ppm2     4 995
ASSI {16842}
  (( segid "BrD " and resid 15   and name HB2 ))
  (( segid "BrD " and resid 15   and name HA  ))
     2 200     1 200     1 200 peak 16842 weight  0 10000E+01 volume  0.62256E+03 ppm1     3 677 ppm2     4 618
ASSI {16882}
  (( segid "BrD " and resid 106  and name HA  ))
  (  segid "BrD " and resid 82   and name HE% )
     4 100     4 100     1 400 peak 16882 weight  0 10000E+01 volume  0 17840E+02 ppm1     4 557 ppm2     7 039
OR {16882}
  (( segid "BrD " and resid 106  and name HA  ))
  (( segid "BrD " and resid 82   and name HZ  ))
ASSI {16892}
  (( segid "BrD " and resid 106  and name HA  ))
  (  segid "BrD " and resid 106  and name HD% )
     2.200     1 200     1.200 peak 16892 weight  0 10000E+01 volume  0 63095E+03 ppm1     4.556 ppm2     7.511
ASSI {16902}
  (( segid "BrD " and resid 106  and name HA  ))
  (  segid "BrD " and resid 106  and name HE% )
     3.000     2 200     2 200 peak 16902 weight  0.10000E+01 volume  0 10621E+03 ppm1     4 558 ppm2     7 634
ASSI {16932}
  (( segid "BrD " and resid 57   and name HA  ))
  (( segid "BrD " and resid 36   and name HA  ))
     5 500     5 500     0 000 peak 16932 weight  0 10000E+01 volume  0 15155E+01 ppm1     4 804 ppm2     5 444
ASSI {16972}
  (( segid "BrD " and resid 106  and name HB2 ))
  (  segid "BrD " and resid 82   and name HE% )
     3 000     2 200     2 200 peak 16972 weight  0 10000E+01 volume  0.99455E+02 ppm1     3 676 ppm2     7 053
ASSI {17032}
  (( segid "BrD " and resid 62   and name HA  ))
  (( segid "BrD " and resid 67   and name HB1 ))
     2 400     1 400     1 400 peak 17032 weight  0 10000E+01 volume  0 47084E+03 ppm1     4 462 ppm2     3.576
ASSI {17072}
  (( segid "BrD " and resid 95   and name HA  ))
  (( segid "BrD " and resid 32   and name HH2 ))
     2.800     2.000     2 000 peak 17072 weight  0 10000E+01 volume  0 16966E+03 ppm1     4 462 ppm2     7 790
ASSI {17192}
  (( segid "BrD " and resid 20   and name HA  ))
  (( segid "BrD " and resid 23   and name HG2 ))
     2.400     1 400     1.400 peak 17192 weight  0.10000E+01 volume  0.43323E+03 ppm1     4 903 ppm2     3 069
ASSI {17342}
  (( segid "BrD " and resid 97   and name HA  ))
  (  segid "BrD " and resid 96   and name HD% )
     2 800     2.000     2 000 peak 17342 weight  0.10000E+01 volume  0 15398E+03 ppm1     4 807 ppm2     7 719
ASSI {17352}
  (( segid "BrD " and resid 34   and name HB2 ))
  (  segid "BrD " and resid 102  and name HD1%)
     3 900     3.800     1 600 peak 17352 weight  0 10000E+01 volume  0 22025E+02 ppm1     3.127 ppm2     1 319
OR {17352}
  (( segid "BrD " and resid 34   and name HB2 ))
  (  segid "BrD " and resid 102  and name HD2%)
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ASSI {17372}
  (( segid "BrD " and resid 34   and name HB1 ))
  (  segid "BrD " and resid 102  and name HD1%)
     4 300     4 300      1.200 peak 17372 weight  0 10000E+01 volume  0.12013E+02 ppm1      4 114 ppm2       1 317
OR {17372}
  (( segid "BrD " and resid 34   and name HB1 ))
  (  segid "BrD " and resid 102  and name HD2%)
ASSI {17452}
  (( segid "BrD " and resid 34   and name HB2 ))
  (  segid "BrD " and resid 34   and name HE% )
     3 800     3 600      1 700 peak 17452 weight  0 10000E+01 volume  0 24806E+02 ppm1      3 122 ppm2       7 774
ASSI {17502}
  (( segid "BrD " and resid 34   and name HA  ))
  (( segid "BrD " and resid 35   and name HA  ))
     4 600     4 600      0 900 peak 17502 weight  0.10000E+01 volume  0 81169E+01 ppm1      5 544 ppm2       4.907
ASSI {17562}
  (  segid "BrD " and resid 81   and name HG2%)
  (( segid "BrD " and resid 34   and name HZ  ))
     3 500     3.100      2 000 peak 17562 weight  0 10000E+01 volume  0 45996E+02 ppm1      0 759 ppm2       7 903
ASSI {17572}
  (  segid "BrD " and resid 81   and name HG2%)
  (  segid "BrD " and resid 34   and name HD% )
     2 500     1 600      1 600 peak 17572 weight  0 10000E+01 volume  0 32265F+03 ppm1      0 761 ppm2       7 706
ASSI {17632}
  (  segid "BrD " and resid 81   and name HG2%)
  (  segid "BrD " and resid 82   and name HD% )
     2 300     1.300      1 300 peak 17632 weight  0 10000E+01 volume  0.48682E+03 ppm1      0 763 ppm2       7 263
ASSI {17642}
  (  segid "BrD " and resid 81   and name HG2%)
  (  segid "BrD " and resid 82   and name HE% )
     2 800     2 000      2 000 peak 17642 weight  0 10000E+01 volume  0 15950E+03 ppm1      0 760 ppm2       7 063
ASSI {17712}
  (( segid "BrD " and resid 33   and name HG1 ))
  (( segid "BrD " and resid 95   and name HA  ))
     3 000     2 200      2 200 peak 17712 weight  0 10000E+01 volume  0 11633E+03 ppm1      0 859 ppm2       4 452
ASSI {17732}
  (( segid "BrD " and resid 33   and name HG1 ))
  (( segid "BrD " and resid 98   and name HB1 ))
     3 400     2.900      2 100 peak 17732 weight  0 10000E+01 volume  0 51004E+02 ppm1      0 859 ppm2       4 020
ASSI {17742}
  (( segid "BrD " and resid 33   and name HG1 ))
  (( segid "BrD " and resid 98   and name HB2 ))
     3 100     2 400      2 400 peak 17742 weight  0 10000E+01 volume  0 94735E+02 ppm1      0 859 ppm2       3 654
ASSI {17762}
  (( segid "BrD " and resid 33   and name HG2 ))
  (( segid "BrD " and resid 95   and name HA  ))
     3 400     2 900      2 100 peak 17762 weight  0 10000E+01 volume  0 53516E+02 ppm1     -0 324 ppm2       4 444
ASSI {17782}
  (( segid "BrD " and resid 33   and name HD1 ))
  (  segid "BrD " and resid 31   and name HB% )
     3 500     3.100      2 000 peak 17782 weight  0 10000E+01 volume  0 42246E+02 ppm1      2 782 ppm2       2 304
ASSI {17902}
  (( segid "BrD " and resid 33   and name HD2 ))
  (  segid "BrD " and resid 34   and name HD% )
     3 900     3 800      1.600 peak 17902 weight  0 10000E+01 volume  0 21155E+02 ppm1      2.190 ppm2       7 707
ASSI {17952}
  (( segid "BrD " and resid 33   and name HB1 ))
  (( segid "BrD " and resid 95   and name HA  ))
     3 800     3 600      1 700 peak 17952 weight  0 10000E+01 volume  0 26579E+02 ppm1      1 055 ppm2       4 443
ASSI {17962}
  (( segid "BrD " and resid 33   and name HB2 ))
  (( segid "BrD " and resid 95   and name HA  ))
     3 900     3 800      1 600 peak 17962 weight  0 10000E+01 volume  0 22889E+02 ppm1     -0 176 ppm2       4 444
ASSI {17982}
  (( segid "BrD " and resid 33   and name HB2 ))
  (  segid "BrD " and resid 34   and name HD% )
     3 700     3 400      1 800 peak 17982 weight  0 10000E+01 volume  0 30273E+02 ppm1     -0 174 ppm2       7.699
ASSI {18012}
  (( segid "BrD " and resid 75   and name HG1 ))
  (( segid "BrD " and resid 71   and name HA  ))
     3 200     2 600      2.300 peak 18012 weight  0 10000E+01 volume  0 74474E+02 ppm1      3 524 ppm2       4 662
ASSI {18052}
  (( segid "BrD " and resid 59   and name HG1 ))
  (( segid "BrD " and resid 59   and name HB2 ))
     2 600     1 700      1 700 peak 18052 weight  0 10000E+01 volume  0 28930E+03 ppm1      3 227 ppm2       2.482
OR {18052}
  (( segid "BrD " and resid 59   and name HG2 ))
  (( segid "BrD " and resid 59   and name HB2 ))
ASSI {18102}
  (( segid "BrD " and resid 75   and name HG2 ))
  (  segid "BrD " and resid 115  and name HD1%)
     4 400     4.400      1.100 peak 18102 weight  0 10000E+01 volume  0 10857E+02 ppm1      3 226 ppm2       1 327
ASSI {18112}
  (( segid "BrD " and resid 59   and name HG2 ))
  (  segid "BrD " and resid 22   and name HD1%)
     4 100     4 100      1.400 peak 18112 weight  0 10000E+01 volume  0.16621E+02 ppm1      3.226 ppm2       1.661
OR {18112}
  (( segid "BrD " and resid 59   and name HG1 ))
  (  segid "BrD " and resid 22   and name HD1%)
ASSI {18122}
  (( segid "BrD " and resid 75   and name HG1 ))
  (( segid "BrD " and resid 115  and name HB1 ))
     3 500     3 100      2 000 peak 18122 weight  0 10000E+01 volume  0.47142E+02 ppm1      3 522 ppm2       2 165
ASSI {18142}
  (( segid "BrD " and resid 75   and name HG1 ))
  (  segid "BrD " and resid 113  and name HB% )
     3 900     3 800      1 600 peak 18142 weight  0.10000E+01 volume  0 23045E+02 ppm1      3 523 ppm2       1 996
ASSI {18282}
  (  segid "BrD " and resid 35   and name HE% )
  (( segid "BrD " and resid 60   and name HB1 ))
     2 800     2 000      2 000 peak 18282 weight  0 10000E+01 volume  0 18338E+03 ppm1      2 782 ppm2       4 972
ASSI {18302}
  (  segid "BrD " and resid 35   and name HE% )
  (( segid "BrD " and resid 59   and name HG2 ))
     3.400     2 900      2 100 peak 18302 weight  0 10000E+01 volume  0 50813E+02 ppm1      2.782 ppm2       3.248
OR {18302}
  (  segid "BrD " and resid 35   and name HE% )
  (( segid "BrD " and resid 59   and name HG1 ))
ASSI {18312}
  (  segid "BrD " and resid 35   and name HE% )
  (( segid "BrD " and resid 34   and name HB2 ))
     3 000     2 200      2 200 peak 18312 weight  0 10000E+01 volume  0.11214E+03 ppm1      2 782 ppm2       3 101
ASSI {18352}
  (  segid "BrD " and resid 35   and name HE% )
  (  segid "BrD " and resid 56   and name HD1%)
     2.800     2.000      2.000 peak 18352 weight  0 10000E+01 volume  0 15609E+03 ppm1      2 782 ppm2       1 539
ASSI {18362}
  (  segid "BrD " and resid 35   and name HE% )
  (( segid "BrD " and resid 57   and name HB1 ))
     2 400     1 400      1 400 peak 18362 weight  0 10000E+01 volume  0.43055E+03 ppm1      2 782 ppm2       2 938
ASSI {18382}
  (  segid "BrD " and resid 35   and name HE% )
  (( segid "BrD " and resid 26   and name HB1 ))
     2 500     1 600      1 600 peak 18382 weight  0 10000E+01 volume  0 29206E+03 ppm1      2 781 ppm2       2 460
ASSI {18492}
  (( segid "BrD " and resid 59   and name HG1 ))
  (  segid "BrD " and resid 74   and name HE% )
     5.000     5 000      0 500 peak 18492 weight  0 10000E+01 volume  0 50782E+01 ppm1      3 226 ppm2       7 552
OR {18492}
  (( segid "BrD " and resid 59   and name HG2 ))
  (  segid "BrD " and resid 74   and name HE% )
ASSI {18542}
  (  segid "BrD " and resid 75   and name HE% )
  (( segid "BrD " and resid 17   and name HB  ))
     3 000     2 200      2 200 peak 18542 weight  0 10000E+01 volume  0.10304E+03 ppm1      2 634 ppm2       4 826
ASSI {18642}
  (  segid "BrD " and resid 75   and name HE% )
  (( segid "BrD " and resid 110  and name HA  ))
     3.400     2 900      2 100 peak 18642 weight  0 10000E+01 volume  0 51911E+02 ppm1      2 634 ppm2       4 427
ASSI {18662}
  (  segid "BrD " and resid 75   and name HE% )
  (( segid "BrD " and resid 74   and name HB1 ))
     2.900     2 100      2 100 peak 18662 weight  0.10000E+01 volume  0 13576E+03 ppm1      2 634 ppm2       3 597
ASSI {18682}
  (  segid "BrD " and resid 75   and name HE% )
  (( segid "BrD " and resid 74   and name HB2 ))
     3.000     2 200      2 200 peak 18682 weight  0 10000E+01 volume  0 11929E+03 ppm1      2 634 ppm2       3 003
ASSI {18722}
  (  segid "BrD " and resid 75   and name HE% )
  (( segid "BrD " and resid 75   and name HB1 ))
     3 700     3 400      1 800 peak 18722 weight  0 10000E+01 volume  0 33115E+02 ppm1      2 634 ppm2       2 906
ASSI {18732}
  (  segid "BrD " and resid 75   and name HE% )
  (( segid "BrD " and resid 75   and name HB2 ))
     2 100     2 100      2 400 peak 18732 weight  0 10000E+01 volume  0 10446E+04 ppm1      2.634 ppm2       2 824
ASSI {18762}
  (  segid "BrD " and resid 75   and name HE% )
  (  segid "BrD " and resid 78   and name HD2%)
     4 900     4 900      0 600 peak 18762 weight  0 10000E+01 volume  0.60943E+01 ppm1      2 634 ppm2       0 676
ASSI {18772}
  (  segid "BrD " and resid 75   and name HE% )
  (  segid "BrD " and resid 14   and name HD1%)
     2 600     1 700      1.700 peak 18772 weight  0 10000E+01 volume  0 27797E+03 ppm1      2.634 ppm2       1 425
OR {18772}
  (  segid "BrD " and resid 75   and name HE% )
  (  segid "BrD " and resid 14   and name HD2%)
ASSI {18782}
  (  segid "BrD " and resid 75   and name HE% )
  (  segid "BrD " and resid 115  and name HD1%)
     2.800     2 000      2 000 peak 18782 weight  0 10000E+01 volume  0.15408E+03 ppm1      2 634 ppm2       1 327
ASSI {18812}
  (  segid "BrD " and resid 75   and name HE% )
  (( segid "BrD " and resid 116  and name HG12))
     3 600     3 200      1 900 peak 18812 weight  0 10000E+01 volume  0.36651E+02 ppm1      2 635 ppm2       1 547
ASSI {18862}
  (  segid "BrD " and resid 75   and name HE% )
  (( segid "BrD " and resid 116  and name HG11))
     4 600     4 600      0 900 peak 18862 weight  0 10000E+01 volume  0 79723E+01 ppm1      2 635 ppm2       1.914
ASSI {18872}
  (  segid "BrD " and resid 75   and name HE% )
  (  segid "BrD " and resid 59   and name HE% )
     3.500     3 100      2 000 peak 18872 weight  0 10000E+01 volume  0.40230E+02 ppm1      2 635 ppm2       1.865
ASSI {18882}
  (  segid "BrD " and resid 75   and name HE% )
  (  segid "BrD " and resid 113  and name HB% )
     2.700     1 800      1 800 peak 18882 weight  0 10000E+01 volume  0 22578E+03 ppm1      2 634 ppm2       1 986
ASSI {18892}
  (  segid "BrD " and resid 75   and name HE% )
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(( segid "BrD " and resid 18   and name HG  ))
   2 400      1 400      1 400 peak 18892 weight  0 10000E+01 volume  0 37764E+03 ppm1      2 636 ppm2      2 250
ASSI {18902}
  (  segid "BrD " and resid 75   and name HE% )
  (( segid "BrD " and resid 115  and name HB1 ))
   2 500      1 600      1 600 peak 18902 weight  0 10000E+01 volume  0 35880E+03 ppm1      2 635 ppm2      2 199
ASSI {18932}
  (  segid "BrD " and resid 75   and name HE% )
  (( segid "BrD " and resid 14   and name HB1 ))
   3 700      3 400      1 800 peak 18932 weight  0 10000E+01 volume  0 29255E+02 ppm1      2 636 ppm2      2.444
ASSI {18952}
  (( segid "BrD " and resid 57   and name HB2 ))
  (( segid "BrD " and resid 37   and name HD1 ))
   3 200      2 600      2 300 peak 18952 weight  0 10000E+01 volume  0 68763E+02 ppm1      2 847 ppm2      4.289
ASSI {18992}
  (( segid "BrD " and resid 57   and name HB2 ))
  (( segid "BrD " and resid 36   and name HA  ))
   3 700      3.400      1 800 peak 18992 weight  0.10000E+01 volume  0.28694E+02 ppm1      2 842 ppm2      5 444
ASSI {19072}
  (( segid "BrD " and resid 31   and name HA  ))
  (( segid "BrD " and resid 34   and name HZ  ))
   3 100      2 400      2 400 peak 19072 weight  0 10000E+01 volume  0 98899E+02 ppm1      5 001 ppm2      7 893
ASSI {19092}
  (( segid "BrD " and resid 31   and name HA  ))
  (( segid "BrD " and resid 30   and name HA  ))
   2 800      2 000      2.000 peak 19092 weight  0 10000E+01 volume  0.15610E+03 ppm1      5 001 ppm2      5 428
ASSI {19172}
  (( segid "BrD " and resid 43   and name HA  ))
  (  segid "BrD " and resid 88   and name HE% )
   3 300      2.700      2 200 peak 19172 weight  0 10000E+01 volume  0.58224E+02 ppm1      5 547 ppm2      7 417
ASSI {19182}
  (( segid "BrD " and resid 43   and name HA  ))
  (( segid "BrD " and resid 44   and name HG1 ))
   2 900      2 100      2 100 peak 19182 weight  0 10000E+01 volume  0 12258E+03 ppm1      5 544 ppm2      2 735
ASSI {19192}
  (( segid "BrD " and resid 43   and name HA  ))
  (( segid "BrD " and resid 44   and name HG2 ))
   3 100      2 400      2 400 peak 19192 weight  0 10000E+01 volume  0 97301E+02 ppm1      5 544 ppm2      2 646
OR {19192}
  (( segid "BrD " and resid 43   and name HA  ))
  (( segid "BrD " and resid 44   and name HB2 ))
ASSI {19202}
  (( segid "BrD " and resid 43   and name HA  ))
  (  segid "BrD " and resid 38   and name HG2%)
   3 500      3 100      2 000 peak 19202 weight  0 10000E+01 volume  0 42319E+02 ppm1      5 544 ppm2      0 799
ASSI {19212}
  (  segid "BrD " and resid 43   and name HB% )
  (( segid "BrD " and resid 42   and name HG1 ))
   3 600      3 200      1 900 peak 19212 weight  0 10000E+01 volume  0.35927E+02 ppm1      1 697 ppm2      2 898
ASSI {19242}
  (  segid "BrD " and resid 43   and name HB% )
  (  segid "BrD " and resid 50   and name HD1%)
   5 400      5 400      0 100 peak 19242 weight  0 10000E+01 volume  0 31463E+01 ppm1      1 697 ppm2      1.148
ASSI {19272}
  (  segid "BrD " and resid 43   and name HB% )
  (( segid "BrD " and resid 39   and name HG1 ))
   3 300      2 700      2 200 peak 19272 weight  0.10000E+01 volume  0 60793E+02 ppm1      1.697 ppm2      2.032
ASSI {19282}
  (  segid "BrD " and resid 43   and name HB% )
  (( segid "BrD " and resid 38   and name HB  ))
   3 000      2 200      2 200 peak 19282 weight  0 10000E+01 volume  0 12013E+03 ppm1      1 697 ppm2      1 790
ASSI {19312}
  (  segid "BrD " and resid 31   and name HB% )
  (  segid "BrD " and resid 25   and name HG1%)
   3 200      2 600      2 300 peak 19312 weight  0 10000E+01 volume  0.68019E+02 ppm1      2 289 ppm2      1 832
ASSI {19352}
  (  segid "BrD " and resid 31   and name HB% )
  (( segid "BrD " and resid 35   and name HB1 ))
   3.400      2 900      2 100 peak 19352 weight  0 10000E+01 volume  0 48169E+02 ppm1      2 289 ppm2      2 841
ASSI {19362}
  (  segid "BrD " and resid 31   and name HB% )
  (( segid "BrD " and resid 28   and name HB1 ))
   2 400      1 400      1.400 peak 19362 weight  0.10000E+01 volume  0 37768E+03 ppm1      2 289 ppm2      3 581
ASSI {19372}
  (  segid "BrD " and resid 31   and name HB% )
  (( segid "BrD " and resid 35   and name HG1 ))
   2 500      1 600      1 600 peak 19372 weight  0 10000E+01 volume  0 30400E+03 ppm1      2 289 ppm2      3.427
ASSI {19382}
  (  segid "BrD " and resid 31   and name HB% )
  (( segid "BrD " and resid 34   and name HB2 ))
   4.200      4 200      1 300 peak 19382 weight  0 10000E+01 volume  0 14651E+02 ppm1      2 289 ppm2      3 134
ASSI {19392}
  (  segid "BrD " and resid 31   and name HB% )
  (( segid "BrD " and resid 28   and name HA  ))
   3 100      2.400      2 400 peak 19392 weight  0 10000E+01 volume  0 87183E+02 ppm1      2 289 ppm2      4 582
ASSI {19422}
  (  segid "BrD " and resid 31   and name HB% )
  (  segid "BrD " and resid 34   and name HE% )
   3 500      3.100      2 000 peak 19422 weight  0 10000E+01 volume  0 44223E+02 ppm1      2 289 ppm2      7.803
ASSI {19482}
  (  segid "BrD " and resid 76   and name HB% )
  (( segid "BrD " and resid 79   and name HB2 ))
   3 300      2.700      2 200 peak 19482 weight  0 10000E+01 volume  0 66817E+02 ppm1      2 092 ppm2      2 662
ASSI {19492}
  (  segid "BrD " and resid 76   and name HB% )
  (( segid "BrD " and resid 80   and name HB2 ))
   2.800      2 000      2 000 peak 19492 weight  0 10000E+01 volume  0 15977E+03 ppm1      2 092 ppm2      2 564
OR {19492}
  (  segid "BrD " and resid 76   and name HB% )
  (( segid "BrD " and resid 80   and name HB1 ))
ASSI {19502}
  (  segid "BrD " and resid 76   and name HB% )
  (( segid "BrD " and resid 80   and name HB2 ))
   2 700      1 800      1 800 peak 19502 weight  0 10000E+01 volume  0 21436E+03 ppm1      2 092 ppm2      2 507
ASSI {19522}
  (  segid "BrD " and resid 76   and name HB% )
  (( segid "BrD " and resid 77   and name HA  ))
   2.800      2.000      2.000 peak 19522 weight  0 10000E+01 volume  0 15327E+03 ppm1      2 092 ppm2      4 963
ASSI {19552}
  (  segid "BrD " and resid 76   and name HB% )
  (( segid "BrD " and resid 51   and name HB2 ))
   2.500      1 600      1 600 peak 19552 weight  0 10000E+01 volume  0 32487E+03 ppm1      2 092 ppm2      1 783
OR {19552}
  (  segid "BrD " and resid 76   and name HB% )
  (( segid "BrD " and resid 51   and name HG2 ))
ASSI {19572}
  (  segid "BrD " and resid 76   and name HB% )
  (  segid "BrD " and resid 116  and name HG2%)
   3.600      3.200      1 900 peak 19572 weight  0 10000E+01 volume  0 35020E+02 ppm1      2 092 ppm2      1 432
ASSI {19582}
  (  segid "BrD " and resid 73   and name HD2%)
  (( segid "BrD " and resid 68   and name HA  ))
   2 800      2 000      2 000 peak 19582 weight  0 10000E+01 volume  0 16681E+03 ppm1      1 500 ppm2      5 143
ASSI {19632}
  (( segid "BrD " and resid 76   and name HA  ))
  (( segid "BrD " and resid 80   and name HG1 ))
   3 100      2 400      2 400 peak 19632 weight  0 10000E+01 volume  0 95067E+02 ppm1      4 656 ppm2      2 327
ASSI {19642}
  (  segid "BrD " and resid 99   and name HB% )
  (( segid "BrD " and resid 34   and name HZ  ))
   2 200      2.200      2.300 peak 19642 weight  0.10000E+01 volume  0 65240E+03 ppm1      2 190 ppm2      7 903
ASSI {19652}
  (  segid "BrD " and resid 99   and name HB% )
  (  segid "BrD " and resid 34   and name HE% )
   2.300      1 300      1 300 peak 19652 weight  0 10000E+01 volume  0 50164E+03 ppm1      2 190 ppm2      7.781
ASSI {19672}
  (  segid "BrD " and resid 99   and name HB% )
  (  segid "BrD " and resid 82   and name HD% )
   2.500      1 600      1.600 peak 19672 weight  0 10000E+01 volume  0 36039E+03 ppm1      2 190 ppm2      7 259
ASSI {19692}
  (  segid "BrD " and resid 99   and name HB% )
  (( segid "BrD " and resid 85   and name HA  ))
   3 100      2 400      2 400 peak 19692 weight  0 10000E+01 volume  0 92786E+02 ppm1      2 190 ppm2      5 005
ASSI {19702}
  (  segid "BrD " and resid 99   and name HB% )
  (( segid "BrD " and resid 100  and name HA  ))
   3.000      2 200      2 200 peak 19702 weight  0 10000E+01 volume  0 10441E+03 ppm1      2 190 ppm2      4 948
ASSI {19752}
  (  segid "BrD " and resid 99   and name HB% )
  (( segid "BrD " and resid 103  and name HG1 ))
   3.000      2 200      2 200 peak 19752 weight  0 10000E+01 volume  0 10256E+03 ppm1      2 190 ppm2      2.613
ASSI {19772}
  (  segid "BrD " and resid 76   and name HB% )
  (( segid "BrD " and resid 79   and name HB1 ))
   3.500      3 100      2 000 peak 19772 weight  0 10000E+01 volume  0 45000E+02 ppm1      2 092 ppm2      2.784
ASSI {19792}
  (( segid "BrD " and resid 99   and name HA  ))
  (( segid "BrD " and resid 34   and name HZ  ))
   2 600      1 700      1 700 peak 19792 weight  0 10000E+01 volume  0.26558E+03 ppm1      4 459 ppm2      7 901
ASSI {19802}
  (( segid "BrD " and resid 99   and name HA  ))
  (  segid "BrD " and resid 34   and name HE% )
   2.700      1 800      1 800 peak 19802 weight  0 10000E+01 volume  0 21467E+03 ppm1      4 459 ppm2      7 771
ASSI {19812}
  (( segid "BrD " and resid 99   and name HA  ))
  (  segid "BrD " and resid 82   and name HE% )
   3.200      2 600      2 300 peak 19812 weight  0 10000E+01 volume  0 71395E+02 ppm1      4 457 ppm2      7 073
ASSI {19822}
  (( segid "BrD " and resid 99   and name HA  ))
  (  segid "BrD " and resid 82   and name HD% )
   2.800      2.000      2.000 peak 19822 weight  0 10000E+01 volume  0 15492E+03 ppm1      4 459 ppm2      7 259
ASSI {19832}
  (( segid "BrD " and resid 99   and name HA  ))
  (( segid "BrD " and resid 100  and name HA  ))
   2.800      2 000      2.000 peak 19832 weight  0 10000E+01 volume  0 16591E+03 ppm1      4 458 ppm2      4 950
ASSI {19842}
  (( segid "BrD " and resid 99   and name HA  ))
  (( segid "BrD " and resid 103  and name HB2 ))
   2 600      1 700      1 700 peak 19842 weight  0.10000E+01 volume  0 24667E+03 ppm1      4 458 ppm2      1.922
ASSI {19882}
  (( segid "BrD " and resid 113  and name HA  ))
  (  segid "BrD " and resid 110  and name HG2%)
   3.600      3 200      1 900 peak 19882 weight  0 10000E+01 volume  0.35803E+02 ppm1      4.903 ppm2      1 222
ASSI {19902}
  (( segid "BrD " and resid 113  and name HA  ))
  (( segid "BrD " and resid 112  and name HB1 ))
   3 400      2 900      2 100 peak 19902 weight  0 10000E+01 volume  0 48759E+02 ppm1      4 903 ppm2      2 670
ASSI {19912}
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(( segid "BrD " and resid 113  and name HA  ))
(( segid "BrD " and resid 110  and name HA  ))
  3 500     3.100     2 000 peak 19912 weight  0 10000E+01 volume  0 44605E+02 ppm1     4 903 ppm2     4.419
ASSI {19922}
  (( segid "BrD " and resid 113  and name HA  ))
  (( segid "BrD " and resid 14   and name HA  ))
  3 100     2 400     2 400 peak 19922 weight  0 10000E+01 volume  0 84488E+02 ppm1     4 903 ppm2     4.663
ASSI {19962}
  (( segid "BrD " and resid 113  and name HA  ))
  (  segid "BrD " and resid 115  and name HD1%)
  4 000     4.000     1 500 peak 19962 weight  0 10000E+01 volume  0 18572E+02 ppm1     4.899 ppm2     1.313
ASSI {19992}
  (  segid "BrD " and resid 113  and name HB% )
  (( segid "BrD " and resid 14   and name HB1 ))
  3 300     2 700     2 200 peak 19992 weight  0 10000E+01 volume  0 60405E+02 ppm1     1.991 ppm2     2 442
ASSI {20032}
  (  segid "BrD " and resid 113  and name HB% )
  (( segid "BrD " and resid 14   and name HG  ))
  2 100     2 100     2 400 peak 20032 weight  0 10000E+01 volume  0 86636E+03 ppm1     1 994 ppm2     2 059
ASSI {20042}
  (  segid "BrD " and resid 113  and name HB% )
  (  segid "BrD " and resid 18   and name HD2%)
  4 200     4 200     1 300 peak 20042 weight  0 10000E+01 volume  0.14101E+02 ppm1     1.993 ppm2     0 408
ASSI {20052}
  (  segid "BrD " and resid 113  and name HB% )
  (  segid "BrD " and resid 115  and name HD1%)
  2 400     1 400     1 400 peak 20052 weight  0 10000E+01 volume  0 47259E+03 ppm1     1 993 ppm2     1 319
ASSI {20072}
  (( segid "BrD " and resid 110  and name HA  ))
  (  segid "BrD " and resid 115  and name HD1%)
  2 500     1 600     1 600 peak 20072 weight  0 10000E+01 volume  0 33630E+03 ppm1     4 409 ppm2     1 319
ASSI {20192}
  (( segid "BrD " and resid 17   and name HB  ))
  (  segid "BrD " and resid 115  and name HD1%)
  3.200     2 600     2.300 peak 20192 weight  0 10000E+01 volume  0 76060E+02 ppm1     4 854 ppm2     1 327
ASSI {20212}
  (( segid "BrD " and resid 17   and name HA  ))
  (  segid "BrD " and resid 21   and name HD1%)
  4.600     4 600     0 900 peak 20212 weight  0 10000E+01 volume  0 88717E+01 ppm1     4 542 ppm2     1 224
ASSI {20242}
  (  segid "BrD " and resid 17   and name HG2%)
  (  segid "BrD " and resid 75   and name HE% )
  2.600     1 700     1 700 peak 20242 weight  0 10000E+01 volume  0 27619E+03 ppm1     1 747 ppm2     2 619
ASSI {20252}
  (  segid "BrD " and resid 17   and name HG2%)
  (( segid "BrD " and resid 21   and name HB  ))
  3.000     2 200     2 200 peak 20252 weight  0 10000E+01 volume  0 10098E+03 ppm1     1 747 ppm2     2 507
ASSI {20272}
  (  segid "BrD " and resid 17   and name HG2%)
  (( segid "BrD " and resid 115  and name HB1 ))
  3 500     3 100     2 000 peak 20272 weight  0 10000E+01 volume  0 46134E+02 ppm1     1 747 ppm2     2 214
ASSI {20292}
  (  segid "BrD " and resid 17   and name HG2%)
  (( segid "BrD " and resid 109  and name HB2 ))
  2 600     1 700     1 700 peak 20292 weight  0 10000E+01 volume  0 25743E+03 ppm1     1 747 ppm2     2 149
ASSI {20302}
  (  segid "BrD " and resid 17   and name HG2%)
  (( segid "BrD " and resid 18   and name HB2 ))
  4 600     4 600     0 900 peak 20302 weight  0 10000E+01 volume  0 84610E+01 ppm1     1.747 ppm2     0 904
ASSI {20312}
  (( segid "BrD " and resid 41   and name HB  ))
  (( segid "BrD " and resid 39   and name HD1 ))
  3 300     2 700     2 200 peak 20312 weight  0 10000E+01 volume  0.67487E+02 ppm1     4 903 ppm2     2 271
ASSI {20332}
  (( segid "BrD " and resid 41   and name HA  ))
  (( segid "BrD " and resid 44   and name HD2 ))
  3 500     3 100     2 000 peak 20332 weight  0 10000E+01 volume  0 42717E+02 ppm1     4.656 ppm2     4 143
ASSI {20382}
  (( segid "BrD " and resid 41   and name HA  ))
  (( segid "BrD " and resid 44   and name HD1 ))
  2.900     2 100     2 100 peak 20382 weight  0.10000E+01 volume  0 13674E+03 ppm1     4.656 ppm2     4 308
ASSI {20532}
  (  segid "BrD " and resid 41   and name HG2%)
  (( segid "BrD " and resid 42   and name HA  ))
  3 400     2 900     2 100 peak 20532 weight  0 10000E+01 volume  0 51387E+02 ppm1     1 845 ppm2     5.062
ASSI {20542}
  (  segid "BrD " and resid 41   and name HG2%)
  (( segid "BrD " and resid 39   and name HG1 ))
  2 600     1 700     1 700 peak 20542 weight  0 10000E+01 volume  0 28354E+03 ppm1     1 844 ppm2     2.019
ASSI {20562}
  (  segid "BrD " and resid 41   and name HG2%)
  (( segid "BrD " and resid 39   and name HD1 ))
  2 900     2 100     2 100 peak 20562 weight  0 10000E+01 volume  0.13596E+03 ppm1     1 844 ppm2     2 296
ASSI {20572}
  (  segid "BrD " and resid 41   and name HG2%)
  (( segid "BrD " and resid 39   and name HB1 ))
  3.200     2 600     2 300 peak 20572 weight  0.10000E+01 volume  0 75085E+02 ppm1     1 845 ppm2     2.466
ASSI {20592}
  (( segid "BrD " and resid 112  and name HG2 ))
  (( segid "BrD " and resid 112  and name HA  ))
  2 400     1 400     1 400 peak 20592 weight  0 10000E+01 volume  0 44748E+03 ppm1     2 832 ppm2     4 585
ASSI {20712}
  (( segid "BrD " and resid 67   and name HA  ))
  (( segid "BrD " and resid 68   and name HA  ))
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  2.800     2.000     2.000 peak 20712 weight  0.10000E+01 volume  0.17530E+03 ppm1     4.656 ppm2     5.111
ASSI {20802}
  (  segid "BrD " and resid 25   and name HG2%)
  (  segid "BrD " and resid 82   and name HE% )
  2 900     2 100     2 100 peak 20802 weight  0 10000E+01 volume  0 13726E+03 ppm1     1 648 ppm2     7 026
OR {20802}
  (  segid "BrD " and resid 25   and name HG2%)
  (( segid "BrD " and resid 82   and name HZ  ))
ASSI {20812}
  (  segid "BrD " and resid 58   and name HG2%)
  (  segid "BrD " and resid 68   and name HE% )
  3.200     2 600     2 300 peak 20812 weight  0 10000E+01 volume  0.69885E+02 ppm1     1 651 ppm2     7 920
ASSI {20852}
  (  segid "BrD " and resid 25   and name HG2%)
  (( segid "BrD " and resid 31   and name HA  ))
  3 400     2 900     2 100 peak 20852 weight  0 10000E+01 volume  0.55839E+02 ppm1     1 649 ppm2     4 980
ASSI {20862}
  (( segid "BrD " and resid 62   and name HD1 ))
  (( segid "BrD " and resid 62   and name HB2 ))
  2 900     2 100     2 100 peak 20862 weight  0 10000E+01 volume  0.12367E+03 ppm1     3.175 ppm2     1 710
ASSI {20872}
  (( segid "BrD " and resid 62   and name HD2 ))
  (( segid "BrD " and resid 62   and name HB2 ))
  3 000     2.200     2 200 peak 20872 weight  0 10000E+01 volume  0.11189E+03 ppm1     2.633 ppm2     1 711
ASSI {20992}
  (( segid "BrD " and resid 62   and name HB1 ))
  (  segid "BrD " and resid 68   and name HE% )
  3 100     2 400     2 400 peak 20992 weight  0 10000E+01 volume  0 97455E+02 ppm1     2 638 ppm2     7 905
ASSI {21082}
  (  segid "BrD " and resid 83   and name HG2%)
  (( segid "BrD " and resid 87   and name HG2 ))
  3 000     2 200     2.200 peak 21082 weight  0 10000E+01 volume  0 11102E+03 ppm1     1 895 ppm2     2 784
ASSI {21142}
  (( segid "BrD " and resid 83   and name HB  ))
  (( segid "BrD " and resid 80   and name HG1 ))
  3 400     2 900     2 100 peak 21142 weight  0 10000E+01 volume  0 55703E+02 ppm1     4 803 ppm2     2 360
ASSI {21192}
  (  segid "BrD " and resid 83   and name HG2%)
  (( segid "BrD " and resid 87   and name HG1 ))
  2.100     1 100     1 100 peak 21192 weight  0 10000E+01 volume  0 10489E+04 ppm1     1 895 ppm2     3 028
ASSI {21202}
  (  segid "BrD " and resid 83   and name HG2%)
  (( segid "BrD " and resid 87   and name HB2 ))
  3 400     2 900     2 100 peak 21202 weight  0 10000E+01 volume  0 47828E+02 ppm1     1 899 ppm2     2 597
ASSI {21292}
  (  segid "BrD " and resid 25   and name HG1%)
  (  segid "BrD " and resid 106  and name HD% )
  2 500     2 500     2.000 peak 21292 weight  0.10000E+01 volume  0 35912E+03 ppm1     1 795 ppm2     7 515
ASSI {21322}
  (  segid "BrD " and resid 25   and name HG1%)
  (  segid "BrD " and resid 82   and name HE% )
  3 500     3 100     2.000 peak 21322 weight  0 10000E+01 volume  0 43989E+02 ppm1     1 795 ppm2     7 026
OR {21322}
  (  segid "BrD " and resid 25   and name HG1%)
  (( segid "BrD " and resid 82   and name HZ  ))
ASSI {21392}
  (( segid "BrD " and resid 25   and name HB  ))
  (  segid "BrD " and resid 102  and name HD1%)
  3 600     3.200     1 900 peak 21392 weight  0 10000E+01 volume  0 35593E+02 ppm1     2 979 ppm2     1 327
OR {21392}
  (( segid "BrD " and resid 25   and name HB  ))
  (  segid "BrD " and resid 102  and name HD2%)
ASSI {21402}
  (( segid "BrD " and resid 25   and name HB  ))
  (  segid "BrD " and resid 78   and name HD2%)
  4.400     4 400     1 100 peak 21402 weight  0 10000E+01 volume  0 11302E+02 ppm1     2.979 ppm2     0 676
ASSI {21422}
  (  segid "BrD " and resid 25   and name HG1%)
  (( segid "BrD " and resid 102  and name HG  ))
  3.500     3 100     2 000 peak 21422 weight  0 10000E+01 volume  0 43674E+02 ppm1     1 795 ppm2     2 157
ASSI {21452}
  (  segid "BrD " and resid 25   and name HG1%)
  (( segid "BrD " and resid 106  and name HB1 ))
  4 300     4 300     1 200 peak 21452 weight  0 10000E+01 volume  0 11856E+02 ppm1     1 796 ppm2     3 907
ASSI {21462}
  (  segid "BrD " and resid 25   and name HG1%)
  (( segid "BrD " and resid 21   and name HA  ))
  2 700     1 800     1.800 peak 21462 weight  0 10000E+01 volume  0 21023E+03 ppm1     1 797 ppm2     4.369
ASSI {21472}
  (  segid "BrD " and resid 25   and name HG1%)
  (( segid "BrD " and resid 102  and name HA  ))
  3 400     2 900     2 100 peak 21472 weight  0 10000E+01 volume  0 48930E+02 ppm1     1 796 ppm2     4.297
ASSI {21562}
  (  segid "BrD " and resid 81   and name HG2%)
  (( segid "BrD " and resid 82   and name HA  ))
  2 900     2.100     2 100 peak 21562 weight  0 10000E+01 volume  0.12812E+03 ppm1     0 760 ppm2     4 753
ASSI {21582}
  (  segid "BrD " and resid 38   and name HG1%)
  (( segid "BrD " and resid 37   and name HA  ))
  3 300     2.700     2 200 peak 21582 weight  0 10000E+01 volume  0.64039E+02 ppm1     1 056 ppm2     4 859
ASSI {21672}
  (  segid "BrD " and resid 81   and name HG1%)
  (  segid "BrD " and resid 34   and name HD% )
  3 400     2 900     2 100 peak 21672 weight  0 10000E+01 volume  0 52778E+02 ppm1     1 056 ppm2     7 706
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ASSI {21702}
  ( segid "BrD " and resid 38   and name HG2%)
  (( segid "BrD " and resid 41   and name HA  ))
    4 900     4 900     0 600 peak 21702 weight  0.10000E+01 volume  0 56291E+01 ppm1    0 808 ppm2    4.646
ASSI {21732}
  ( segid "BrD " and resid 81   and name HG2%)
  ( segid "BrD " and resid 56   and name HD2%)
    2.600     1 700     1 700 peak 21732 weight  0 10000E+01 volume  0 28103E+03 ppm1    0.760 ppm2    1.238
ASSI {21742}
  ( segid "BrD " and resid 81   and name HG2%)
  ( segid "BrD " and resid 102  and name HD1%)
    3 900     3 800     1 600 peak 21742 weight  0 10000E+01 volume  0 21895E+02 ppm1    0 760 ppm2    1.319
OR {21742}
  ( segid "BrD " and resid 81   and name HG2%)
  ( segid "BrD " and resid 102  and name HD2%)
ASSI {21752}
  ( segid "BrD " and resid 81   and name HG2%)
  (( segid "BrD " and resid 84   and name HB2 ))
    3 000     2 200     2 200 peak 21752 weight  0 10000E+01 volume  0 11571E+03 ppm1    0 763 ppm2    3 296
ASSI {21772}
  (( segid "BrD " and resid 81   and name HB  ))
  ( segid "BrD " and resid 78   and name HD2%)
    3 200     2 600     2 300 peak 21772 weight  0 10000E+01 volume  0 80152E+02 ppm1    2 042 ppm2    0 683
ASSI {21802}
  (( segid "BrD " and resid 81   and name HA  ))
  (( segid "BrD " and resid 80   and name HB1 ))
    3 900     3 800     1 600 peak 21802 weight  0 10000E+01 volume  0 23614E+02 ppm1    3 719 ppm2    2 564
OR {21802}
  (( segid "BrD " and resid 81   and name HA  ))
  (( segid "BrD " and resid 80   and name HB2 ))
ASSI {21812}
  (( segid "BrD " and resid 81   and name HA  ))
  (( segid "BrD " and resid 80   and name HB1 ))
    3 600     3 200     1 900 peak 21812 weight  0 10000E+01 volume  0 37077E+02 ppm1    3 719 ppm2    2 597
ASSI {21902}
  (( segid "BrD " and resid 49   and name HA  ))
  ( segid "BrD " and resid 50   and name HD1%)
    4 100     4 100     1 400 peak 21902 weight  0 10000E+01 volume  0 17504E+02 ppm1    4 656 ppm2    1 140
ASSI {21952}
  ( segid "BrD " and resid 50   and name HD1%)
  (( segid "BrD " and resid 88   and name HB1 ))
    2 400     1 400     1 400 peak 21952 weight  0 10000E+01 volume  0 36864E+03 ppm1    1.155 ppm2    3.535
ASSI {21972}
  ( segid "BrD " and resid 50   and name HD1%)
  (( segid "BrD " and resid 46   and name HA  ))
    4 100     4 100     1 400 peak 21972 weight  0 10000E+01 volume  0 16984E+02 ppm1    1 155 ppm2    4 151
ASSI {22022}
  ( segid "BrD " and resid 50   and name HD1%)
  ( segid "BrD " and resid 88   and name HD% )
    3 100     2 400     2 400 peak 22022 weight  0 10000E+01 volume  0 82494E+02 ppm1    1 155 ppm2    7 606
ASSI {22042}
  (( segid "BrD " and resid 50   and name HB  ))
  (( segid "BrD " and resid 51   and name HB1 ))
    4 800     4 800     0 700 peak 22042 weight  0 10000E+01 volume  0 67010E+01 ppm1    1 797 ppm2    1 966
OR {22042}
  (( segid "BrD " and resid 50   and name HB  ))
  (( segid "BrD " and resid 51   and name HG1 ))
ASSI {22132}
  (( segid "BrD " and resid 50   and name HA  ))
  ( segid "BrD " and resid 49   and name HG2%)
    2 500     1 600     1 600 peak 22132 weight  0 10000E+01 volume  0 30657E+03 ppm1    4 506 ppm2    1 570
ASSI {22142}
  (( segid "BrD " and resid 50   and name HA  ))
  ( segid "BrD " and resid 49   and name HG1%)
    3 800     3 600     1 700 peak 22142 weight  0 10000E+01 volume  0 27941E+02 ppm1    4 506 ppm2    1 646
ASSI {22212}
  ( segid "BrD " and resid 50   and name HG2%)
  (( segid "BrD " and resid 51   and name HB1 ))
    4 000     4 000     1 500 peak 22212 weight  0 10000E+01 volume  0 20287E+02 ppm1    1 007 ppm2    1 954
ASSI {22222}
  (( segid "BrD " and resid 84   and name HA  ))
  ( segid "BrD " and resid 83   and name HG2%)
    4 100     4 100     1 400 peak 22222 weight  0 10000E+01 volume  0 17290E+02 ppm1    4 903 ppm2    1 913
ASSI {22232}
  (( segid "BrD " and resid 84   and name HA  ))
  (( segid "BrD " and resid 87   and name HG1 ))
    3 500     3 100     2 000 peak 22232 weight  0 10000E+01 volume  0.41523E+02 ppm1    4.904 ppm2    3 010
ASSI {22242}
  (( segid "BrD " and resid 84   and name HA  ))
  (( segid "BrD " and resid 88   and name HB1 ))
    3 100     2 400     2 400 peak 22242 weight  0.10000E+01 volume  0.82426E+02 ppm1    4.904 ppm2    3 533
ASSI {22322}
  ( segid "BrD " and resid 69   and name HG1%)
  (( segid "BrD " and resid 66   and name HA  ))
    2 800     2 000     2 000 peak 22322 weight  0 10000E+01 volume  0.17920E+03 ppm1    1 551 ppm2    4 989
ASSI {22332}
  ( segid "BrD " and resid 69   and name HG1%)
  (( segid "BrD " and resid 68   and name HA  ))
    5.000     5 000     0 500 peak 22332 weight  0.10000E+01 volume  0 51283E+01 ppm1    1 551 ppm2    5 141
ASSI {22372}
  ( segid "BrD " and resid 69   and name HG2%)
  (( segid "BrD " and resid 66   and name HB1 ))
    4.000     4 000     1 500 peak 22372 weight  0 10000E+01 volume  0 19974E+02 ppm1    1 425 ppm2    2.726
ASSI {22382}
  ( segid "BrD " and resid 69   and name HG2%)
  (( segid "BrD " and resid 11   and name HB2 ))
    3 100     2 400     2 400 peak 22382 weight  0 10000E+01 volume  0.94687E+02 ppm1    1.425 ppm2    2 612
ASSI {22452}
  ( segid "BrD " and resid 69   and name HG2%)
  ( segid "BrD " and resid 63   and name HD1%)
    2 400     1.400     1.400 peak 22452 weight  0 10000E+01 volume  0 42940E+03 ppm1    1 425 ppm2    1 659
ASSI {22482}
  ( segid "BrD " and resid 49   and name HG2%)
  (( segid "BrD " and resid 50   and name HG12))
    4.000     4.000     1 500 peak 22482 weight  0.10000E+01 volume  0.18478E+02 ppm1    1 548 ppm2    0 808
ASSI {22492}
  ( segid "BrD " and resid 49   and name HG2%)
  (( segid "BrD " and resid 87   and name HA  ))
    4 900     4 900     0 600 peak 22492 weight  0.10000E+01 volume  0 59811E+01 ppm1    1 549 ppm2    4 854
ASSI {22552}
  ( segid "BrD " and resid 49   and name HG1%)
  (( segid "BrD " and resid 50   and name HG12))
    4.800     4.800     0 700 peak 22552 weight  0 10000E+01 volume  0.66665E+01 ppm1    1 647 ppm2    0.835
ASSI {22592}
  (( segid "BrD " and resid 57   and name HG2 ))
  (( segid "BrD " and resid 36   and name HA  ))
    3 500     3 100     2 000 peak 22592 weight  0 10000E+01 volume  0 41488E+02 ppm1    2 016 ppm2    5 446
ASSI {22612}
  (( segid "BrD " and resid 42   and name HA  ))
  ( segid "BrD " and resid 43   and name HB% )
    4 300     4 300     1 200 peak 22612 weight  0 10000E+01 volume  0.12059E+02 ppm1    5 050 ppm2    1 710
ASSI {22632}
  (( segid "BrD " and resid 42   and name HA  ))
  (( segid "BrD " and resid 44   and name HD1 ))
    4 200     4 200     1 300 peak 22632 weight  0 10000E+01 volume  0.14713E+02 ppm1    5 051 ppm2    4 337
ASSI {22642}
  (( segid "BrD " and resid 42   and name HA  ))
  (( segid "BrD " and resid 43   and name HA  ))
    4 000     4 000     1.500 peak 22642 weight  0.10000E+01 volume  0 19305E+02 ppm1    5 051 ppm2    5 550
ASSI {22682}
  (( segid "BrD " and resid 117  and name HA  ))
  (( segid "BrD " and resid 116  and name HA  ))
    3 200     2.600     2.300 peak 22682 weight  0 10000E+01 volume  0 76840E+02 ppm1    5 148 ppm2    4 826
ASSI {22722}
  (( segid "BrD " and resid 117  and name HA  ))
  ( segid "BrD " and resid 116  and name HD1%)
    4 300     4 300     1 200 peak 22722 weight  0 10000E+01 volume  0 13070E+02 ppm1    5 149 ppm2    1 409
OR {22722}
  (( segid "BrD " and resid 117  and name HA  ))
  ( segid "BrD " and resid 116  and name HG2%)
ASSI {22732}
  (( segid "BrD " and resid 7    and name HB1 ))
  (( segid "BrD " and resid 8    and name HD2 ))
    2 800     2 000     2 000 peak 22732 weight  0 10000E+01 volume  0 18127E+03 ppm1    2 636 ppm2    4 287
ASSI {22742}
  (( segid "BrD " and resid 37   and name HA  ))
  (( segid "BrD " and resid 38   and name HA  ))
    3 900     3 800     1.600 peak 22742 weight  0 10000E+01 volume  0.21223E+02 ppm1    4 853 ppm2    4 167
ASSI {22752}
  (( segid "BrD " and resid 37   and name HA  ))
  (( segid "BrD " and resid 38   and name HB  ))
    5 500     5 500     0.000 peak 22752 weight  0 10000E+01 volume  0.13492E+00 ppm1    4 853 ppm2    1 759
ASSI {22852}
  (( segid "BrD " and resid 59   and name HB2 ))
  ( segid "BrD " and resid 56   and name HD2%)
    3 300     2.700     2 200 peak 22852 weight  0 10000E+01 volume  0 58772E+02 ppm1    2 486 ppm2    1 246
ASSI {22882}
  (( segid "BrD " and resid 8    and name HD2 ))
  (( segid "BrD " and resid 8    and name HA  ))
    3.300     2 700     2 200 peak 22882 weight  0 10000E+01 volume  0 65959E+02 ppm1    4 261 ppm2    5 021
ASSI {22892}
  (( segid "BrD " and resid 8    and name HD1 ))
  (( segid "BrD " and resid 8    and name HA  ))
    2.800     2 000     2 000 peak 22892 weight  0 10000E+01 volume  0.15205E+03 ppm1    4 407 ppm2    5 019
ASSI {22932}
  (( segid "BrD " and resid 37   and name HD1 ))
  (( segid "BrD " and resid 37   and name HA  ))
    3 000     2 200     2.200 peak 22932 weight  0 10000E+01 volume  0 11242E+03 ppm1    4 261 ppm2    4.859
ASSI {22952}
  (( segid "BrD " and resid 44   and name HD2 ))
  (( segid "BrD " and resid 42   and name HA  ))
    3 600     3.200     1.900 peak 22952 weight  0 10000E+01 volume  0 34019E+02 ppm1    4 114 ppm2    5 046
ASSI {22962}
  (( segid "BrD " and resid 91   and name HD2 ))
  (( segid "BrD " and resid 93   and name HB2 ))
    3 000     2 200     2 200 peak 22962 weight  0.10000E+01 volume  0.11249E+03 ppm1    4 409 ppm2    4.745
ASSI {22992}
  (( segid "BrD " and resid 11   and name HD1 ))
  (( segid "BrD " and resid 11   and name HB1 ))
    2.500     1 600     1 600 peak 22992 weight  0.10000E+01 volume  0 33828E+03 ppm1    4 457 ppm2    2 945
ASSI {23012}
  (( segid "BrD " and resid 8    and name HD1 ))
  (( segid "BrD " and resid 8    and name HB1 ))
    3.300     2.700     2.200 peak 23012 weight  0 10000E+01 volume  0.56548E+02 ppm1    4 409 ppm2    2.849
ASSI {23022}
  (( segid "BrD " and resid 44   and name HD1 ))
  (( segid "BrD " and resid 44   and name HG1 ))
    2 100     1 100     1 100 peak 23022 weight  0 10000E+01 volume  0 84503E+03 ppm1    4 311 ppm2    2 727
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ASSI {23062}
  (( segid "BrD " and resid 37   and name HD1 ))
  (( segid "BrD " and resid 37   and name HB2 ))
    3 200    2.600    2 300 peak 23062 weight  0 10000E+01 volume  0 68384E+02 ppm1     4 261 ppm2     2 287
ASSI {23082}
  (( segid "BrD " and resid 91   and name HD1 ))
  (( segid "BrD " and resid 91   and name HG1 ))
    2 600    1 700    1 700 peak 23082 weight  0 10000E+01 volume  0 26320E+03 ppm1     4 557 ppm2     2 784
ASSI {23092}
  (( segid "BrD " and resid 44   and name HD2 ))
  (( segid "BrD " and resid 44   and name HG1 ))
    2 300    1 300    1 300 peak 23092 weight  0 10000E+01 volume  0 51719E+03 ppm1     4 114 ppm2     2.735
ASSI {23102}
  (( segid "BrD " and resid 44   and name HD2 ))
  (( segid "BrD " and resid 44   and name HG2 ))
    2 300    1 300    1 300 peak 23102 weight  0 10000E+01 volume  0 54971E+03 ppm1     4 114 ppm2     2 654
ASSI {23112}
  (( segid "BrD " and resid 11   and name HD1 ))
  (( segid "BrD " and resid 11   and name HG1 ))
    2 600    1 700    1 700 peak 23112 weight  0 10000E+01 volume  0 26059E+03 ppm1     4 454 ppm2     2 648
ASSI {23122}
  (( segid "BrD " and resid 44   and name HD2 ))
  (( segid "BrD " and resid 44   and name HB1 ))
    2 700    1.800    1 800 peak 23122 weight  0 10000E+01 volume  0 21568E+03 ppm1     4 124 ppm2     2 973
ASSI {23202}
  (( segid "BrD " and resid 44   and name HG2 ))
  (( segid "BrD " and resid 41   and name HA  ))
    3 200    2 600    2 300 peak 23202 weight  0 10000E+01 volume  0.75568E+02 ppm1     2 635 ppm2     4.666
ASSI {23242}
  (( segid "BrD " and resid 11   and name HG1 ))
  (  segid "BrD " and resid 69   and name HG1%)
    3 200    2 600    2 300 peak 23242 weight  0 10000E+01 volume  0 73085E+02 ppm1     2 635 ppm2     1 547
ASSI {23272}
  (( segid "BrD " and resid 11   and name HG1 ))
  (  segid "BrD " and resid 14   and name HD2%)
    3 500    3 100    2 000 peak 23272 weight  0 10000E+01 volume  0 45861E+02 ppm1     2 635 ppm2     1 376
OR {23272}
  (( segid "BrD " and resid 11   and name HG1 ))
  (  segid "BrD " and resid 14   and name HD1%)
ASSI {23292}
  (( segid "BrD " and resid 91   and name HG1 ))
  (( segid "BrD " and resid 89   and name HA  ))
    4 600    4 600    0 900 peak 23292 weight  0 10000E+01 volume  0 80378E+01 ppm1     2 784 ppm2     5 646
ASSI {23372}
  (( segid "BrD " and resid 9    and name HD1 ))
  (  segid "BrD " and resid 14   and name HD1%)
    3 700    3 400    1 800 peak 23372 weight  0 10000E+01 volume  0 32255E+02 ppm1     3 768 ppm2     1 425
OR {23372}
  (( segid "BrD " and resid 9    and name HD1 ))
  (  segid "BrD " and resid 14   and name HD2%)
ASSI {23402}
  (( segid "BrD " and resid 100  and name HA  ))
  (( segid "BrD " and resid 86   and name HE1 ))
    3 500    3 100    2 000 peak 23402 weight  0 10000E+01 volume  0 44085E+02 ppm1     4 952 ppm2     3 093
ASSI {23422}
  (( segid "BrD " and resid 9    and name HB2 ))
  (( segid "BrD " and resid 8    and name HA  ))
    3 000    2 200    2 200 peak 23422 weight  0 10000E+01 volume  0 11322E+03 ppm1     2 388 ppm2     5 029
ASSI {23472}
  (( segid "BrD " and resid 6    and name HA  ))
  (( segid "BrD " and resid 6    and name HG1 ))
    1 900    0 900    0 900 peak 23472 weight  0 10000E+01 volume  0 18609E+04 ppm1     4 952 ppm2     2 214
ASSI {23572}
  (( segid "BrD " and resid 11   and name HB2 ))
  (( segid "BrD " and resid 10   and name HA  ))
    3 600    3 200    1 900 peak 23572 weight  0 10000E+01 volume  0.38586E+02 ppm1     2 585 ppm2     5 477
ASSI {23592}
  (( segid "BrD " and resid 12   and name HA  ))
  (( segid "BrD " and resid 11   and name HA  ))
    4 600    4 600    0 900 peak 23592 weight  0 10000E+01 volume  0.79375E+01 ppm1     5 297 ppm2     4 948
ASSI {23602}
  (( segid "BrD " and resid 29   and name HG1 ))
  (( segid "BrD " and resid 27   and name HA  ))
    3 900    3 800    1 600 peak 23602 weight  0 10000E+01 volume  0.21350E+02 ppm1     2 978 ppm2     5 022
ASSI {23632}
  (( segid "BrD " and resid 13   and name HB1 ))
  (( segid "BrD " and resid 113  and name HA  ))
    2 700    1 800    1 800 peak 23632 weight  0 10000E+01 volume  0.21427E+03 ppm1     2 733 ppm2     4 920
ASSI {23642}
  (( segid "BrD " and resid 13   and name HG2 ))
  (( segid "BrD " and resid 113  and name HA  ))
    3 200    2 600    2 300 peak 23642 weight  0.10000E+01 volume  0 71312E+02 ppm1     2 978 ppm2     4.920
ASSI {23652}
  (( segid "BrD " and resid 13   and name HB1 ))
  (( segid "BrD " and resid 12   and name HB2 ))
    2 900    2.100    2 100 peak 23652 weight  0 10000E+01 volume  0 14282E+03 ppm1     2 732 ppm2     3 359
ASSI {23672}
  (( segid "BrD " and resid 14   and name HA  ))
  (  segid "BrD " and resid 18   and name HD2%)
    3 300    2 700    2 200 peak 23672 weight  0 10000E+01 volume  0 64900E+02 ppm1     4 654 ppm2     0 409
ASSI {23712}
  (( segid "BrD " and resid 111  and name HA  ))
  (  segid "BrD " and resid 110  and name HG2%)
    2 400    1 400    1 400 peak 23712 weight  0 10000E+01 volume  0 44849E+03 ppm1     4.656 ppm2     1 246
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ASSI {23732}
  (( segid "BrD " and resid 14   and name HB2 ))
  (  segid "BrD " and resid 14   and name HD2%)
    2.200    1 200    1 200 peak 23732 weight  0 10000E+01 volume  0 70287E+03 ppm1     2 142 ppm2     1 402
OR {23732}
  (( segid "BrD " and resid 14   and name HB2 ))
  (  segid "BrD " and resid 14   and name HD1%)
ASSI {23762}
  (  segid "BrD " and resid 14   and name HD2%)
  (( segid "BrD " and resid 70   and name HA  ))
    3 100    2 400    2 400 peak 23762 weight  0.10000E+01 volume  0 94978E+02 ppm1     1 401 ppm2     5 359
ASSI {23802}
  (  segid "BrD " and resid 14   and name HD2%)
  (( segid "BrD " and resid 15   and name HB1 ))
    3 800    3.600    1 700 peak 23802 weight  0 10000E+01 volume  0 26555E+02 ppm1     1 401 ppm2     3 785
ASSI {23842}
  (  segid "BrD " and resid 14   and name HD2%)
  (  segid "BrD " and resid 75   and name HE% )
    2 600    1 700    1 700 peak 23842 weight  0 10000E+01 volume  0 23698E+03 ppm1     1 401 ppm2     2 619
ASSI {23882}
  (( segid "BrD " and resid 18   and name HA  ))
  (( segid "BrD " and resid 17   and name HB  ))
    3 500    3.100    2 000 peak 23882 weight  0.10000E+01 volume  0.41356E+02 ppm1     3 867 ppm2     4 867
ASSI {23922}
  (( segid "BrD " and resid 18   and name HB1 ))
  (  segid "BrD " and resid 63   and name HD2%)
    3 900    3 800    1 600 peak 23922 weight  0 10000E+01 volume  0 21833E+02 ppm1     2 144 ppm2     1 492
ASSI {23972}
  (( segid "BrD " and resid 18   and name HB2 ))
  (  segid "BrD " and resid 74   and name HE% )
    3 200    2 600    2 300 peak 23972 weight  0 10000E+01 volume  0 77951E+02 ppm1     0 911 ppm2     7 533
ASSI {23982}
  (( segid "BrD " and resid 18   and name HB2 ))
  (  segid "BrD " and resid 74   and name HD% )
    3.700    3 400    1 800 peak 23982 weight  0.10000E+01 volume  0 32246E+02 ppm1     0 911 ppm2     7 014
ASSI {24022}
  (( segid "BrD " and resid 18   and name HG  ))
  (  segid "BrD " and resid 115  and name HD1%)
    4 500    4.500    1 000 peak 24022 weight  0 10000E+01 volume  0 94731E+01 ppm1     2 290 ppm2     1 317
ASSI {24032}
  (  segid "BrD " and resid 18   and name HD2%)
  (( segid "BrD " and resid 75   and name HA  ))
    3.400    2 900    2 100 peak 24032 weight  0 10000E+01 volume  0 52852E+02 ppm1     0 415 ppm2     4 541
ASSI {24202}
  (  segid "BrD " and resid 18   and name HD1%)
  (( segid "BrD " and resid 17   and name HB  ))
    3.900    3 800    1 600 peak 24202 weight  0 10000E+01 volume  0 21965E+02 ppm1     1 056 ppm2     4.859
ASSI {24232}
  (  segid "BrD " and resid 18   and name HD1%)
  (( segid "BrD " and resid 15   and name HB1 ))
    3.700    3 400    1 800 peak 24232 weight  0 10000E+01 volume  0 32596E+02 ppm1     1 056 ppm2     3 801
ASSI {24262}
  (  segid "BrD " and resid 18   and name HD1%)
  (  segid "BrD " and resid 78   and name HD2%)
    3 500    3 100    2 000 peak 24262 weight  0 10000E+01 volume  0 41978E+02 ppm1     1 056 ppm2     0 676
ASSI {24272}
  (  segid "BrD " and resid 18   and name HD1%)
  (( segid "BrD " and resid 69   and name HA  ))
    3 400    2 900    2 100 peak 24272 weight  0.10000E+01 volume  0 49516E+02 ppm1     1 057 ppm2     4 692
ASSI {24302}
  (( segid "BrD " and resid 63   and name HA  ))
  (( segid "BrD " and resid 68   and name HB2 ))
    3 300    2 700    2 200 peak 24302 weight  0 10000E+01 volume  0 61304E+02 ppm1     5 294 ppm2     3 557
ASSI {24452}
  (( segid "BrD " and resid 63   and name HG  ))
  (( segid "BrD " and resid 68   and name HB2 ))
    3 400    2 900    2.100 peak 24452 weight  0 10000E+01 volume  0 51423E+02 ppm1     2 437 ppm2     3 516
ASSI {24462}
  (( segid "BrD " and resid 63   and name HG  ))
  (( segid "BrD " and resid 15   and name HA  ))
    2.500    2 500    2 000 peak 24462 weight  0 10000E+01 volume  0.29838E+03 ppm1     2 437 ppm2     4 645
ASSI {24482}
  (  segid "BrD " and resid 63   and name HD1%)
  (( segid "BrD " and resid 18   and name HA  ))
    3 600    3 200    1 900 peak 24482 weight  0 10000E+01 volume  0.38413E+02 ppm1     1 649 ppm2     3 878
ASSI {24512}
  (  segid "BrD " and resid 63   and name HD1%)
  (( segid "BrD " and resid 68   and name HB2 ))
    2 900    2 100    2 100 peak 24512 weight  0 10000E+01 volume  0.12238E+03 ppm1     1 649 ppm2     3 527
ASSI {24542}
  (  segid "BrD " and resid 63   and name HD1%)
  (  segid "BrD " and resid 74   and name HD% )
    3 200    2 600    2 300 peak 24542 weight  0 10000E+01 volume  0 76917E+02 ppm1     1 648 ppm2     7 006
ASSI {24682}
  (( segid "BrD " and resid 19   and name HA  ))
  (  segid "BrD " and resid 22   and name HD2%)
    3.100    2.400    2 400 peak 24682 weight  0 10000E+01 volume  0 84277E+02 ppm1     4 311 ppm2     1 588
ASSI {24702}
  (( segid "BrD " and resid 19   and name HA  ))
  (( segid "BrD " and resid 19   and name HE1 ))
    3 100    2.400    2 400 peak 24702 weight  0 10000E+01 volume  0 84024E+02 ppm1     4 310 ppm2     3 544
ASSI {24782}
  (( segid "BrD " and resid 19   and name HG1 ))
  (  segid "BrD " and resid 15   and name HE% )
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   3.300    2.700     2.200 peak 24782 weight  0.10000E+01 volume  0.57590E+02 ppm1   1.895 ppm2   7.487
ASSI {24832}
  (( segid "BrD " and resid 19   and name HD1 ))
  (  segid "BrD " and resid 15   and name HE% )
   2 400    1 400     1 400 peak 24832 weight  0.10000E+01 volume  0 37891E+03 ppm1   2 191 ppm2   7 469
ASSI {24842}
  (( segid "BrD " and resid 19   and name HD1 ))
  (  segid "BrD " and resid 63   and name HD1%)
   2.200    2 200     2 300 peak 24842 weight  0 10000E+01 volume  0 74438E+03 ppm1   2 191 ppm2   1 654
ASSI {24882}
  (( segid "BrD " and resid 23   and name HG1 ))
  (( segid "BrD " and resid 19   and name HG1 ))
   2 600    1 700     1 700 peak 24882 weight  0 10000E+01 volume  0.24553E+03 ppm1   3 124 ppm2   1 888
ASSI {24892}
  (( segid "BrD " and resid 23   and name HG2 ))
  (( segid "BrD " and resid 19   and name HG1 ))
   2 500    1 600     1 600 peak 24892 weight  0.10000E+01 volume  0 29588E+03 ppm1   3.068 ppm2   1 888
ASSI {25012}
  (( segid "BrD " and resid 21   and name HB  ))
  (  segid "BrD " and resid 106  and name HD% )
   2 400    1 400     1 400 peak 25012 weight  0 10000E+01 volume  0 42303E+03 ppm1   2 486 ppm2   7 519
ASSI {25022}
  (( segid "BrD " and resid 21   and name HG12))
  (  segid "BrD " and resid 106  and name HD% )
   4 300    4 300     1 200 peak 25022 weight  0 10000E+01 volume  0 12393E+02 ppm1   1.648 ppm2   7 511
ASSI {25072}
  (( segid "BrD " and resid 21   and name HG12))
  (  segid "BrD " and resid 17   and name HG2%)
   2 800    2 000     2 000 peak 25072 weight  0 10000E+01 volume  0 15768E+03 ppm1   1 648 ppm2   1 746
ASSI {25082}
  (( segid "BrD " and resid 21   and name HG11))
  (  segid "BrD " and resid 17   and name HG2%)
   2 200    1 200     1 200 peak 25082 weight  0 10000E+01 volume  0.65857E+03 ppm1   2 336 ppm2   1 746
ASSI {25092}
  (( segid "BrD " and resid 21   and name HG11))
  (  segid "BrD " and resid 102  and name HD2%)
   3 800    3 600     1 700 peak 25092 weight  0.10000E+01 volume  0 25380E+02 ppm1   2 338 ppm2   1 322
OR {25092}
  (( segid "BrD " and resid 21   and name HG11))
  (  segid "BrD " and resid 102  and name HD1%)
ASSI {25102}
  (( segid "BrD " and resid 21   and name HG12))
  (( segid "BrD " and resid 20   and name HB1 ))
   3.300    2 700     2 200 peak 25102 weight  0.10000E+01 volume  0 61127E+02 ppm1   1 648 ppm2   4 647
ASSI {25132}
  (( segid "BrD " and resid 62   and name HG1 ))
  (( segid "BrD " and resid 62   and name HG2 ))
   2 200    1 200     1 200 peak 25132 weight  0 10000E+01 volume  0 61439E+03 ppm1   2 336 ppm2   1.498
ASSI {25192}
  (  segid "BrD " and resid 21   and name HD1%)
  (  segid "BrD " and resid 102  and name HD2%)
   2 800    2 000     2 000 peak 25192 weight  0 10000E+01 volume  0 17249E+03 ppm1   1.205 ppm2   1 312
ASSI {25202}
  (  segid "BrD " and resid 21   and name HD1%)
  (( segid "BrD " and resid 18   and name HB2 ))
   3 400    2 900     2 100 peak 25202 weight  0 10000E+01 volume  0 54202E+02 ppm1   1 205 ppm2   0 902
ASSI {25272}
  (  segid "BrD " and resid 21   and name HG2%)
  (  segid "BrD " and resid 106  and name HE% )
   2 800    2 000     2 000 peak 25272 weight  0 10000E+01 volume  0 17880E+03 ppm1   1 599 ppm2   7 638
ASSI {25302}
  (  segid "BrD " and resid 21   and name HG2%)
  (( segid "BrD " and resid 82   and name HZ  ))
   3 500    3 100     2 000 peak 25302 weight  0 10000E+01 volume  0 42795E+02 ppm1   1 599 ppm2   6 998
ASSI {25312}
  (  segid "BrD " and resid 101  and name HG2%)
  (( segid "BrD " and resid 30   and name HA  ))
   3 500    3 100     2 000 peak 25312 weight  0 10000E+01 volume  0 43138E+02 ppm1   1 599 ppm2   5 444
ASSI {25322}
  (( segid "BrD " and resid 101  and name HA  ))
  (( segid "BrD " and resid 100  and name HA  ))
   3 400    2 900     2 100 peak 25322 weight  0 10000E+01 volume  0 52950E+02 ppm1   4 261 ppm2   4 948
ASSI {25332}
  (( segid "BrD " and resid 101  and name HA  ))
  (( segid "BrD " and resid 100  and name HB1 ))
   3.100    2 400     2 400 peak 25333 weight  0 10000E+01 volume  0 82741E+02 ppm1   4 261 ppm2   3 475
ASSI {25342}
  (( segid "BrD " and resid 101  and name HB  ))
  (( segid "BrD " and resid 30   and name HB2 ))
   3.200    2 600     2 300 peak 25342 weight  0 10000E+01 volume  0 74692E+02 ppm1   2 536 ppm2   4 525
ASSI {25352}
  (( segid "BrD " and resid 101  and name HB  ))
  (( segid "BrD " and resid 30   and name HB1 ))
   2 900    2 100     2 100 peak 25352 weight  0 10000E+01 volume  0.14018E+03 ppm1   2 536 ppm2   4 932
ASSI {25362}
  (( segid "BrD " and resid 101  and name HB  ))
  (  segid "BrD " and resid 102  and name HD1%)
   3 500    3 100     2 000 peak 25362 weight  0 10000E+01 volume  0 47210E+02 ppm1   2 536 ppm2   1 311
ASSI {25382}
  (( segid "BrD " and resid 98   and name HA  ))
  (  segid "BrD " and resid 102  and name HD1%)
   5 100    5 100     0 400 peak 25382 weight  0 10000E+01 volume  0 46968E+01 ppm1   4 804 ppm2   1 311
ASSI {25402}
  (( segid "BrD " and resid 98   and name HA  ))
  (( segid "BrD " and resid 30   and name HA  ))
   3 300    2 700     2 200 peak 25402 weight  0 10000E+01 volume  0 66772E+02 ppm1   4.804 ppm2   5.444
ASSI {25412}
  (( segid "BrD " and resid 98   and name HA  ))
  (  segid "BrD " and resid 34   and name HE% )
   3 700    3.400     1.800 peak 25412 weight  0.10000E+01 volume  0 30316E+02 ppm1   4 804 ppm2   7 779
ASSI {25422}
  (( segid "BrD " and resid 98   and name HB1 ))
  (( segid "BrD " and resid 30   and name HB1 ))
   2 900    2 100     2 100 peak 25422 weight  0.10000E+01 volume  0 12678E+03 ppm1   4.013 ppm2   4 933
ASSI {25442}
  (( segid "BrD " and resid 98   and name HB1 ))
  (( segid "BrD " and resid 30   and name HB2 ))
   3 300    2.700     2.200 peak 25442 weight  0 10000E+01 volume  0.62906E+02 ppm1   4 015 ppm2   4 533
ASSI {25452}
  (( segid "BrD " and resid 85   and name HB2 ))
  (  segid "BrD " and resid 99   and name HB% )
   2 500    1 600     1 600 peak 25452 weight  0 10000E+01 volume  0 29534E+03 ppm1   3 620 ppm2   2.206
ASSI {25462}
  (( segid "BrD " and resid 85   and name HB1 ))
  (  segid "BrD " and resid 99   and name HB% )
   2 800    2 000     2.000 peak 25462 weight  0 10000E+01 volume  0 15410E+03 ppm1   3 916 ppm2   2 206
ASSI {25502}
  (( segid "BrD " and resid 98   and name HB2 ))
  (( segid "BrD " and resid 34   and name HZ  ))
   2 900    2 100     2 100 peak 25502 weight  0.10000E+01 volume  0 12121E+03 ppm1   3 670 ppm2   7 893
ASSI {25512}
  (( segid "BrD " and resid 85   and name HB2 ))
  (  segid "BrD " and resid 34   and name HE% )
   2 400    1 400     1 400 peak 25512 weight  0 10000E+01 volume  0 45042E+03 ppm1   3 620 ppm2   7 779
ASSI {25522}
  (( segid "BrD " and resid 85   and name HB1 ))
  (  segid "BrD " and resid 34   and name HE% )
   2 500    1 600     1 600 peak 25522 weight  0 10000E+01 volume  0 32323E+03 ppm1   3 917 ppm2   7 778
ASSI {25562}
  (  segid "BrD " and resid 101  and name HD1%)
  (( segid "BrD " and resid 30   and name HB2 ))
   3 500    3 100     2 000 peak 25562 weight  0.10000E+01 volume  0 41073E+02 ppm1   1 551 ppm2   4 532
ASSI {25572}
  (  segid "BrD " and resid 101  and name HD1%)
  (( segid "BrD " and resid 30   and name HB1 ))
   3 000    2 200     2 200 peak 25572 weight  0 10000E+01 volume  0 10658E+03 ppm1   1 549 ppm2   4 932
ASSI {25582}
  (  segid "BrD " and resid 21   and name HG2%)
  (  segid "BrD " and resid 18   and name HD2%)
   3 600    3 200     1 900 peak 25582 weight  0.10000E+01 volume  0 38225E+02 ppm1   1.599 ppm2   0 408
ASSI {25642}
  (  segid "BrD " and resid 21   and name HG2%)
  (( segid "BrD " and resid 24   and name HG2 ))
   3 600    3.200     1 900 peak 25642 weight  0 10000E+01 volume  0 38422E+02 ppm1   1 599 ppm2   3 069
ASSI {25652}
  (  segid "BrD " and resid 21   and name HG2%)
  (( segid "BrD " and resid 109  and name HE2 ))
   4 000    4 000     1 500 peak 25652 weight  0 10000E+01 volume  0 20266E+02 ppm1   1 599 ppm2   3 012
ASSI {25722}
  (  segid "BrD " and resid 21   and name HG2%)
  (( segid "BrD " and resid 109  and name HB2 ))
   2 700    1 800     1 800 peak 25722 weight  0 10000E+01 volume  0 18743E+03 ppm1   1 599 ppm2   2 157
ASSI {25752}
  (  segid "BrD " and resid 101  and name HD1%)
  (( segid "BrD " and resid 102  and name HB1 ))
   3 100    2 400     2.400 peak 25752 weight  0 10000E+01 volume  0 84468E+02 ppm1   1 549 ppm2   1 970
ASSI {25812}
  (( segid "BrD " and resid 110  and name HB  ))
  (  segid "BrD " and resid 116  and name HD1%)
   2 300    1 300     1 300 peak 25812 weight  0 10000E+01 volume  0 55301E+03 ppm1   2.338 ppm2   1 410
ASSI {25822}
  (( segid "BrD " and resid 110  and name HG11))
  (  segid "BrD " and resid 78   and name HD2%)
   4.000    4 000     1 500 peak 25822 weight  0.10000E+01 volume  0 19996E+02 ppm1   1 697 ppm2   0.676
ASSI {25842}
  (  segid "BrD " and resid 110  and name HD1%)
  (( segid "BrD " and resid 75   and name HA  ))
   3 100    2 400     2 400 peak 25842 weight  0.10000E+01 volume  0 86474E+02 ppm1   1 154 ppm2   4 511
ASSI {25852}
  (  segid "BrD " and resid 110  and name HG2%)
  (( segid "BrD " and resid 114  and name HA1 ))
   4.200    4 200     1 300 peak 25852 weight  0 10000E+01 volume  0 14960E+02 ppm1   1 254 ppm2   4 569
ASSI {25952}
  (  segid "BrD " and resid 110  and name HG2%)
  (  segid "BrD " and resid 107  and name HD% )
   3.200    2 600     2.300 peak 25952 weight  0 10000E+01 volume  0.71378E+02 ppm1   1 251 ppm2   7 789
ASSI {26002}
  (  segid "BrD " and resid 110  and name HD1%)
  (  segid "BrD " and resid 106  and name HE% )
   2 500    1 600     1 600 peak 26002 weight  0.10000E+01 volume  0 29658E+03 ppm1   1 155 ppm2   7 638
ASSI {26012}
  (  segid "BrD " and resid 110  and name HD1%)
  (  segid "BrD " and resid 106  and name HD% )
   2.700    1 800     1 800 peak 26012 weight  0 10000E+01 volume  0 22034E+03 ppm1   1 155 ppm2   7 529
ASSI {26082}
  (  segid "BrD " and resid 110  and name HD1%)
  (( segid "BrD " and resid 115  and name HB1 ))
   2 300    1.300     1.300 peak 26082 weight  0 10000E+01 volume  0 51339E+03 ppm1   1 154 ppm2   2 182
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ASSI {26092}
  (  segid "BrD " and resid 110  and name HG2%)
  (( segid "BrD " and resid 111  and name HB1 ))
    3 400     2 900     2 100 peak 26092 weight  0 10000E+01 volume  0 52641E+02 ppm1     1 254 ppm2      2.493
ASSI {26122}
  (  segid "BrD " and resid 110  and name HG2%)
  (( segid "BrD " and resid 116  and name HG11))
    3 700     3 400     1 800 peak 26122 weight  0 10000E+01 volume  0 30456E+02 ppm1     1 254 ppm2      1 918
ASSI {26132}
  (  segid "BrD " and resid 110  and name HD1%)
  (( segid "BrD " and resid 116  and name HG11))
    3 300     2.700     2 200 peak 26132 weight  0 10000E+01 volume  0.58180E+02 ppm1     1 154 ppm2      1 918
ASSI {26142}
  (  segid "BrD " and resid 110  and name HD1%)
  (  segid "BrD " and resid 113  and name HB% )
    2 400     1.400     1 400 peak 26142 weight  0 10000E+01 volume  0.40630E+03 ppm1     1 154 ppm2      1 978
ASSI {26212}
  (  segid "BrD " and resid 116  and name HG2%)
  (( segid "BrD " and resid 117  and name HA  ))
    4 200     4.200     1 300 peak 26212 weight  0 10000E+01 volume  0 13762E+02 ppm1     1 401 ppm2      5 168
ASSI {26222}
  (  segid "BrD " and resid 116  and name HG2%)
  (( segid "BrD " and resid 79   and name HB2 ))
    3 200     2 600     2 300 peak 26222 weight  0 10000E+01 volume  0 79045E+02 ppm1     1 401 ppm2      2 662
ASSI {26242}
  (  segid "BrD " and resid 116  and name HG2%)
  (( segid "BrD " and resid 115  and name HB1 ))
    3 800     3 600     1 700 peak 26242 weight  0 10000E+01 volume  0 25845E+02 ppm1     1.401 ppm2      2.175
ASSI {26252}
  (  segid "BrD " and resid 116  and name HG2%)
  (( segid "BrD " and resid 116  and name HG11))
    2 700     1 800     1 800 peak 26252 weight  0 10000E+01 volume  0 22212E+03 ppm1     1 401 ppm2      1 906
ASSI {26262}
  (  segid "BrD " and resid 116  and name HG2%)
  (  segid "BrD " and resid 110  and name HD1%)
    2 400     2 400     2 100 peak 26262 weight  0 10000E+01 volume  0 45578E+03 ppm1     1 401 ppm2      1 140
ASSI {26322}
  (  segid "BrD " and resid 116  and name HD1%)
  (( segid "BrD " and resid 107  and name HA  ))
    3 200     2 600     2 300 peak 26322 weight  0 10000E+01 volume  0 76194E+02 ppm1     1 401 ppm2      4 427
ASSI {26372}
  (  segid "BrD " and resid 116  and name HD1%)
  (( segid "BrD " and resid 75   and name HG1 ))
    3 200     2 600     2.300 peak 26372 weight  0 10000E+01 volume  0.79388E+02 ppm1     1 401 ppm2      3 508
ASSI {26382}
  (  segid "BrD " and resid 116  and name HD1%)
  (( segid "BrD " and resid 79   and name HB2 ))
    3 400     2 900     2 100 peak 26382 weight  0.10000E+01 volume  0 54400E+02 ppm1     1.401 ppm2      2.662
ASSI {26402}
  (  segid "BrD " and resid 116  and name HD1%)
  (( segid "BrD " and resid 110  and name HG11))
    2 600     1 700     1.700 peak 26402 weight  0 10000E+01 volume  0 24061E+03 ppm1     1 401 ppm2      1 718
ASSI {26412}
  (  segid "BrD " and resid 116  and name HD1%)
  (( segid "BrD " and resid 110  and name HG12))
    2.100     1 100     1 100 peak 26412 weight  0 10000E+01 volume  0 93798E+03 ppm1     1 401 ppm2      1 637
ASSI {26432}
  (  segid "BrD " and resid 116  and name HD1%)
  (( segid "BrD " and resid 78   and name HB2 ))
    2 400     2 400     2 100 peak 26432 weight  0 10000E+01 volume  0 39159E+03 ppm1     1 399 ppm2      1 078
ASSI {26472}
  (  segid "BrD " and resid 116  and name HD1%)
  (  segid "BrD " and resid 78   and name HD2%)
    4 900     4 900     0.600 peak 26472 weight  0 10000E+01 volume  0.55118E+01 ppm1     1 399 ppm2      0 680
ASSI {26482}
  (  segid "BrD " and resid 116  and name HD1%)
  (  segid "BrD " and resid 110  and name HG2%)
    2.000     1 000     1 000 peak 26482 weight  0 10000E+01 volume  0 13707E+04 ppm1     1.399 ppm2      1 237
ASSI {26502}
  (  segid "BrD " and resid 63   and name HD2%)
  (( segid "BrD " and resid 60   and name HA  ))
    2.300     1 300     1 300 peak 26502 weight  0 10000E+01 volume  0 60749E+03 ppm1     1 501 ppm2      4 818
ASSI {26522}
  (( segid "BrD " and resid 116  and name HB  ))
  (( segid "BrD " and resid 115  and name HB1 ))
    4 400     4 400     1 100 peak 26522 weight  0 10000E+01 volume  0 11059E+02 ppm1     2 432 ppm2      2 200
ASSI {26532}
  (( segid "BrD " and resid 116  and name HB  ))
  (  segid "BrD " and resid 110  and name HG2%)
    3 600     3.200     1 900 peak 26532 weight  0 10000E+01 volume  0 35446E+02 ppm1     2 409 ppm2      1.263
ASSI {26542}
  (( segid "BrD " and resid 116  and name HB  ))
  (  segid "BrD " and resid 110  and name HD1%)
    3 300     2 700     2.200 peak 26542 weight  0 10000E+01 volume  0.65125E+02 ppm1     2.409 ppm2      1.149
ASSI {26682}
  (( segid "BrD " and resid 103  and name HG2 ))
  (( segid "BrD " and resid 104  and name HA  ))
    3 300     2 700     2.200 peak 26682 weight  0 10000E+01 volume  0 56609E+02 ppm1     2 519 ppm2      4.679
ASSI {26692}
  (( segid "BrD " and resid 94   and name HG1 ))
  (( segid "BrD " and resid 93   and name HB1 ))
    5 400     5 400     0 100 peak 26692 weight  0 10000E+01 volume  0 32972E+01 ppm1     3 127 ppm2      5 038
OR {26692}
  (( segid "BrD " and resid 94   and name HG1 ))
  (( segid "BrD " and resid 93   and name HA  ))
ASSI {26702}
  (( segid "BrD " and resid 94   and name HG1 ))
  (( segid "BrD " and resid 95   and name HA  ))
    3.700     3 400     1 800 peak 26702 weight  0 10000E+01 volume  0.33522E+02 ppm1     3 132 ppm2      4.448
ASSI {26752}
  (( segid "BrD " and resid 94   and name HG1 ))
  (( segid "BrD " and resid 97   and name HD1 ))
    2 600     1 700     1.700 peak 26752 weight  0.10000E+01 volume  0 26306E+03 ppm1     3 127 ppm2      2 401
ASSI {26872}
  (( segid "BrD " and resid 86   and name HD1 ))
  (( segid "BrD " and resid 87   and name HG1 ))
    2.700     1 800     1 800 peak 26872 weight  0 10000E+01 volume  0 22393E+03 ppm1     1 892 ppm2      3 028
ASSI {26902}
  (( segid "BrD " and resid 36   and name HG1 ))
  (( segid "BrD " and resid 57   and name HG2 ))
    3 500     3 100     2 000 peak 26902 weight  0 10000E+01 volume  0.44296E+02 ppm1     2 781 ppm2      2.003
ASSI {26922}
  (( segid "BrD " and resid 37   and name HB1 ))
  (( segid "BrD " and resid 54   and name HA  ))
    4 000     4 000     1 500 peak 26922 weight  0 10000E+01 volume  0 19758E+02 ppm1     2 930 ppm2      5 542
ASSI {26952}
  (( segid "BrD " and resid 37   and name HG1 ))
  (( segid "BrD " and resid 36   and name HA  ))
    5 300     5 300     0 200 peak 26952 weight  0 10000E+01 volume  0 36066E+01 ppm1     2 733 ppm2      5 444
ASSI {26962}
  (( segid "BrD " and resid 112  and name HG2 ))
  (( segid "BrD " and resid 111  and name HG2 ))
    3 400     2 900     2 100 peak 26962 weight  0 10000E+01 volume  0.56268E+02 ppm1     2 815 ppm2      1 898
ASSI {26972}
  (( segid "BrD " and resid 61   and name HB2 ))
  (  segid "BrD " and resid 58   and name HG2%)
    3 000     2 200     2.200 peak 26972 weight  0 10000E+01 volume  0 11517E+03 ppm1     2 684 ppm2      1 644
ASSI {27022}
  (( segid "BrD " and resid 89   and name HA  ))
  (( segid "BrD " and resid 93   and name HB2 ))
    3 700     3 400     1 800 peak 27022 weight  0 10000E+01 volume  0.31951E+02 ppm1     5.642 ppm2      4 745
ASSI {27032}
  (( segid "BrD " and resid 89   and name HB1 ))
  (( segid "BrD " and resid 96   and name HB2 ))
    3 300     2 700     2.200 peak 27032 weight  0 10000E+01 volume  0 59751E+02 ppm1     3 669 ppm2      3 117
ASSI {27082}
  (( segid "BrD " and resid 100  and name HB2 ))
  (  segid "BrD " and resid 101  and name HD1%)
    4 000     4 000     1 500 peak 27082 weight  0 10000E+01 volume  0 18249E+02 ppm1     3 421 ppm2      1 572
OR {27082}
  (( segid "BrD " and resid 100  and name HB2 ))
  (  segid "BrD " and resid 101  and name HG2%)
ASSI {27092}
  (( segid "BrD " and resid 100  and name HB2 ))
  (( segid "BrD " and resid 101  and name HA  ))
    4 000     4.000     1.500 peak 27092 weight  0.10000E+01 volume  0 18330E+02 ppm1     3 423 ppm2      4 265
ASSI {27102}
  (( segid "BrD " and resid 100  and name HB2 ))
  (( segid "BrD " and resid 101  and name HG11))
    2 700     1 800     1 800 peak 27102 weight  0 10000E+01 volume  0.20958E+03 ppm1     3 423 ppm2      2 458
ASSI {27112}
  (( segid "BrD " and resid 100  and name HB2 ))
  (  segid "BrD " and resid 99   and name HB% )
    3 400     2 900     2 100 peak 27112 weight  0 10000E+01 volume  0.49005E+02 ppm1     3 423 ppm2      2 206
ASSI {27142}
  (( segid "BrD " and resid 80   and name HD1 ))
  (( segid "BrD " and resid 77   and name HA  ))
    3 100     2 400     2 400 peak 27142 weight  0 10000E+01 volume  0 85246E+02 ppm1     3 962 ppm2      4 963
ASSI {27172}
  (( segid "BrD " and resid 80   and name HD2 ))
  (( segid "BrD " and resid 84   and name HB2 ))
    4 100     4 100     1 400 peak 27172 weight  0 10000E+01 volume  0 16098E+02 ppm1     3 913 ppm2      3.276
ASSI {27192}
  (( segid "BrD " and resid 80   and name HD2 ))
  (( segid "BrD " and resid 83   and name HB  ))
    3 400     2.900     2 100 peak 27192 weight  0 10000E+01 volume  0 47687E+02 ppm1     3 912 ppm2      4 808
ASSI {27202}
  (( segid "BrD " and resid 80   and name HD2 ))
  (( segid "BrD " and resid 52   and name HA  ))
    3 900     3.800     1.600 peak 27202 weight  0 10000E+01 volume  0 23078E+02 ppm1     3 902 ppm2      5 583
ASSI {27322}
  (( segid "BrD " and resid 56   and name HG  ))
  (  segid "BrD " and resid 81   and name HG1%)
    3 400     2 900     2.100 peak 27322 weight  0 10000E+01 volume  0 49600E+02 ppm1     2 339 ppm2      1 079
ASSI {27342}
  (( segid "BrD " and resid 55   and name HB1 ))
  (( segid "BrD " and resid 34   and name HA  ))
    3.300     2.700     2 200 peak 27342 weight  0.10000E+01 volume  0 66937E+02 ppm1     2 979 ppm2      5 539
ASSI {27362}
  (( segid "BrD " and resid 55   and name HB1 ))
  (  segid "BrD " and resid 81   and name HG1%)
    3 900     3 800     1 600 peak 27362 weight  0 10000E+01 volume  0 24126E+02 ppm1     2 979 ppm2      1 075
ASSI {27372}
  (( segid "BrD " and resid 38   and name HA  ))
  (( segid "BrD " and resid 39   and name HA  ))
    3 500     3 100     2 000 peak 27372 weight  0 10000E+01 volume  0 46123E+02 ppm1     4 163 ppm2      4 972
ASSI {27392}
  (( segid "BrD " and resid 55   and name HB1 ))
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(( segid "BrD " and resid 36   and name HA  ))
    3 400     2 900     2 100 peak 27392 weight  0.10000E+01 volume  0 54954E+02 ppm1     2 979 ppm2     5 442
ASSI {27442}
  (  segid "BrD " and resid 69   and name HG1%)
  (  segid "BrD " and resid 18   and name HD1%)
    2 400     2 400     2.100 peak 27442 weight  0 10000E+01 volume  0 37353E+03 ppm1     1 547 ppm2     1 091
ASSI {27452}
  (  segid "BrD " and resid 22   and name HD2%)
  (  segid "BrD " and resid 25   and name HG1%)
    2 500     1 600     1 600 peak 27452 weight  0.10000E+01 volume  0 30318E+03 ppm1     1 599 ppm2     1 788
ASSI {27472}
  (  segid "BrD " and resid 22   and name HD2%)
  (( segid "BrD " and resid 25   and name HB  ))
    3.400     2 900     2 100 peak 27472 weight  0 10000E+01 volume  0 54052E+02 ppm1     1.599 ppm2     3 003
ASSI {27492}
  (  segid "BrD " and resid 22   and name HD2%)
 .(( segid "BrD " and resid 60   and name HA  ))
    2 300     1 300     1 300 peak 27492 weight  0 10000E+01 volume  0 56630E+03 ppm1     1 599 ppm2     4.809
ASSI {27552}
  (  segid "BrD " and resid 22   and name HD2%)
  (  segid "BrD " and resid 74   and name HE% )
    2 300     2 300     2 200 peak 27552 weight  0 10000E+01 volume  0 54070E+03 ppm1     1.599 ppm2     7.529
ASSI {27572}
  (  segid "BrD " and resid 22   and name HD1%)
  (( segid "BrD " and resid 60   and name HB1 ))
    3 200     2 600     2 300 peak 27572 weight  0 10000E+01 volume  0 80681E+02 ppm1     1 645 ppm2     4 990
ASSI {27582}
  (  segid "BrD " and resid 22   and name HD1%)
  (  segid "BrD " and resid 74   and name HE% )
    2 200     1 200     1 200 peak 27582 weight  0 10000E+01 volume  0 62438E+03 ppm1     1 646 ppm2     7 529
ASSI {27632}
  (  segid "BrD " and resid 73   and name HD1%)
  (( segid "BrD " and resid 68   and name HA  ))
    2 500     1 600     1 600 peak 27632 weight  0 10000E+01 volume  0 31070E+03 ppm1     1 549 ppm2     5 143
ASSI {27662}
  (  segid "BrD " and resid 73   and name HD1%)
  (( segid "BrD " and resid 70   and name HB2 ))
    3 100     2 400     2 400 peak 27662 weight  0 10000E+01 volume  0 86052E+02 ppm1     1 549 ppm2     4 362
ASSI {27692}
  (  segid "BrD " and resid 73   and name HD2%)
  (  segid "BrD " and resid 76   and name HB% )
    2 800     2.000     2 000 peak 27692 weight  0 10000E+01 volume  0 17686E+03 ppm1     1 500 ppm2     2 106
ASSI {27712}
  (( segid "BrD " and resid 35   and name HA  ))
  (( segid "BrD " and resid 56   and name HB2 ))
    2 100     1 100     1 100 peak 27712 weight  0 10000E+01 volume  0 10158E+04 ppm1     4 900 ppm2     2 004
ASSI {27722}
  (( segid "BrD " and resid 48   and name HA  ))
  (  segid "BrD " and resid 49   and name HG1%)
    3.000     2 200     2 200 peak 27722 weight  0 10000E+01 volume  0 11137E+03 ppm1     4 803 ppm2     1 652
ASSI {27772}
  (( segid "BrD " and resid 73   and name HB2 ))
  (( segid "BrD " and resid 70   and name HB2 ))
    3 400     2 900     2 100 peak 27772 weight  0 10000E+01 volume  0.55069E+02 ppm1     2 487 ppm2     4 377
ASSI {27822}
  (( segid "BrD " and resid 78   and name HA  ))
  (( segid "BrD " and resid 77   and name HB1 ))
    3 800     3 600     1 700 peak 27822 weight  0 10000E+01 volume  0 26285E+02 ppm1     3 967 ppm2     3 312
ASSI {27842}
  (( segid "BrD " and resid 78   and name HB2 ))
  (( segid "BrD " and resid 116  and name HG11))
    3 700     3 400     1 800 peak 27842 weight  0.10000E+01 volume  0 31985E+02 ppm1     1 056 ppm2     1 954
ASSI {27872}
  (( segid "BrD " and resid 78   and name HB2 ))
  (( segid "BrD " and resid 79   and name HA  ))
    4 100     4 100     1 400 peak 27872 weight  0.10000E+01 volume  0 17221E+02 ppm1     1 056 ppm2     4 411
ASSI {27882}
  (( segid "BrD " and resid 78   and name HG  ))
  (( segid "BrD " and resid 75   and name HA  ))
    5 500     5 500     0 000 peak 27882 weight  0 10000E+01 volume  0 22274E+01 ppm1     1 254 ppm2     4 509
ASSI {27892}
  (( segid "BrD " and resid 78   and name HG  ))
  (( segid "BrD " and resid 82   and name HZ  ))
    2 500     2 500     2 000 peak 27892 weight  0 10000E+01 volume  0 30077E+03 ppm1     1 254 ppm2     7.047
OR {27892}
  (( segid "BrD " and resid 78   and name HG  ))
  (  segid "BrD " and resid 82   and name HE% )
ASSI {27912}
  (( segid "BrD " and resid 78   and name HB2 ))
  (  segid "BrD " and resid 106  and name HD% )
    3 600     3 200     1 900 peak 27912 weight  0 10000E+01 volume  0 34865E+02 ppm1     1.056 ppm2     7 532
ASSI {27942}
  (  segid "BrD " and resid 78   and name HD1%)
  (  segid "BrD " and resid 106  and name HE% )
    2 600     1 700     1 700 peak 27942 weight  0 10000E+01 volume  0 24618E+03 ppm1     0 760 ppm2     7 635
ASSI {27982}
  (  segid "BrD " and resid 78   and name HD2%)
  (  segid "BrD " and resid 106  and name HD% )
    2 200     1 200     1 200 peak 27982 weight  0.10000E+01 volume  0 76393E+03 ppm1     0.662 ppm2     7 528
ASSI {27992}
  (  segid "BrD " and resid 78   and name HD2%)
  (( segid "BrD " and resid 82   and name HZ  ))
    2 100     1 100     1 100 peak 27992 weight  0 10000E+01 volume  0 83417E+03 ppm1     0 662 ppm2     7 031
OR {27992}
  (  segid "BrD " and resid 78   and name HD2%)
  (  segid "BrD " and resid 82   and name HE% )
ASSI {28012}
  (  segid "BrD " and resid 78   and name HD2%)
  (  segid "BrD " and resid 106  and name HE% )
    2.900     2 100     2 100 peak 28012 weight  0 10000E+01 volume  0 14234E+03 ppm1     0.662 ppm2     7 637
ASSI {28032}
  (  segid "BrD " and resid 78   and name HD1%)
  (( segid "BrD " and resid 22   and name HA  ))
    3 500     3.100     2 000 peak 28032 weight  0 10000E+01 volume  0 43609E+02 ppm1     0 761 ppm2     4 727
ASSI {28062}
  (  segid "BrD " and resid 78   and name HD1%)
  (( segid "BrD " and resid 75   and name HA  ))
    3.500     3 100     2 000 peak 28062 weight  0 10000E+01 volume  0.46405E+02 ppm1     0 761 ppm2     4 525
ASSI {28102}
  (  segid "BrD " and resid 78   and name HD1%)
  (( segid "BrD " and resid 106  and name HB1 ))
    4 700     4 700     0 800 peak 28102 weight  0 10000E+01 volume  0 77501E+01 ppm1     0.761 ppm2     3 918
ASSI {28122}
  (  segid "BrD " and resid 78   and name HD2%)
  (( segid "BrD " and resid 106  and name HB2 ))
    2.900     2 100     2.100 peak 28122 weight  0 10000E+01 volume  0.14435E+03 ppm1     0.662 ppm2     3 703
ASSI {28132}
  (  segid "BrD " and resid 78   and name HD2%)
  (( segid "BrD " and resid 106  and name HB1 ))
    2 900     2 100     2 100 peak 28132 weight  0 10000E+01 volume  0 12278E+03 ppm1     0 662 ppm2     3.919
ASSI {28192}
  (  segid "BrD " and resid 78   and name HD1%)
  (( segid "BrD " and resid 81   and name HB  ))
    2 700     1 800     1 800 peak 28192 weight  0 10000E+01 volume  0 18524E+03 ppm1     0 760 ppm2     2 043
ASSI {28202}
  (  segid "BrD " and resid 78   and name HD1%)
  (  segid "BrD " and resid 22   and name HD2%)
    2 500     1 600     1 600 peak 28202 weight  0 10000E+01 volume  0.29008E+03 ppm1     0 761 ppm2     1 590
ASSI {28232}
  (  segid "BrD " and resid 78   and name HD1%)
  (  segid "BrD " and resid 18   and name HD2%)
    3 300     2 700     2 200 peak 28232 weight  0 10000E+01 volume  0 64808E+02 ppm1     0 760 ppm2     0 424
ASSI {28262}
  (  segid "BrD " and resid 56   and name HD2%)
  (  segid "BrD " and resid 74   and name HE% )
    4 100     4 100     1 400 peak 28262 weight  0.10000E+01 volume  0 17777E+02 ppm1     1 254 ppm2     7 534
ASSI {28272}
  (  segid "BrD " and resid 56   and name HD2%)
  (  segid "BrD " and resid 82   and name HE% )
    3 400     2 900     2 100 peak 28272 weight  0 10000E+01 volume  0 54803E+02 ppm1     1.253 ppm2     7 041
OR {28272}
  (  segid "BrD " and resid 56   and name HD2%)
  (( segid "BrD " and resid 82   and name HZ  ))
ASSI {28292}
  (  segid "BrD " and resid 56   and name HD2%)
  (( segid "BrD " and resid 55   and name HA  ))
    3 500     3 100     2 000 peak 28292 weight  0 10000E+01 volume  0 41030E+02 ppm1     1 254 ppm2     5 371
ASSI {28322}
  (  segid "BrD " and resid 56   and name HD2%)
  (( segid "BrD " and resid 26   and name HA  ))
    3.100     2 400     2 400 peak 28322 weight  0 10000E+01 volume  0.83493E+02 ppm1     1 254 ppm2     4 509
ASSI {28342}
  (  segid "BrD " and resid 56   and name HD2%)
  (( segid "BrD " and resid 22   and name HA  ))
    3 000     2.200     2.200 peak 28342 weight  0 10000E+01 volume  0.99805E+02 ppm1     1 251 ppm2     4 733
ASSI {28352}
  (  segid "BrD " and resid 56   and name HD2%)
  (( segid "BrD " and resid 78   and name HA  ))
    3.800     3 600     1 700 peak 28352 weight  0 10000E+01 volume  0 27666E+02 ppm1     1 254 ppm2     3 996
ASSI {28372}
  (  segid "BrD " and resid 56   and name HD2%)
  (( segid "BrD " and resid 25   and name HB  ))
    3 500     3.100     2 000 peak 28372 weight  0 10000E+01 volume  0.41722E+02 ppm1     1 254 ppm2     3 003
ASSI {28402}
  (( segid "BrD " and resid 56   and name HB1 ))
  (( segid "BrD " and resid 35   and name HG1 ))
    3.800     3 600     1 700 peak 28402 weight  0 10000E+01 volume  0 28628E+02 ppm1     2.684 ppm2     3 451
ASSI {28412}
  (( segid "BrD " and resid 56   and name HB2 ))
  (( segid "BrD " and resid 35   and name HG1 ))
    4 000     4 000     1 500 peak 28412 weight  0 10000E+01 volume  0 20241E+02 ppm1     1 993 ppm2     3.443
ASSI {28442}
  (( segid "BrD " and resid 102  and name HB1 ))
  (  segid "BrD " and resid 82   and name HE% )
    2.900     2 100     2 100 peak 28442 weight  0 10000E+01 volume  0 13708E+03 ppm1     1 993 ppm2     7 064
ASSI {28472}
  (( segid "BrD " and resid 102  and name HB2 ))
  (  segid "BrD " and resid 34   and name HE% )
    3.200     2 600     2 300 peak 28472 weight  0 10000E+01 volume  0 70904E+02 ppm1     1 842 ppm2     7 778
ASSI {28502}
  (( segid "BrD " and resid 102  and name HB2 ))
  (  segid "BrD " and resid 81   and name HG2%)
    3.600     3 200     1.900 peak 28502 weight  0.10000E+01 volume  0 34445E+02 ppm1     1 842 ppm2     0 766
ASSI {28532}
  (( segid "BrD " and resid 102  and name HG  ))
  (  segid "BrD " and resid 82   and name HE% )
    2.500     1 600     1 600 peak 28532 weight  0.10000E+01 volume  0 29286E+03 ppm1     2 141 ppm2     7 041
ASSI {28562}
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  (  segid "BrD " and resid 102  and name HD2%)
  (  segid "BrD " and resid 82   and name HD% )
     3 600     3 200      1 900 peak 28562 weight  0 10000E+01 volume  0 38923E+02 ppm1     1.303 ppm2     7 245
ASSI {28582}
  (  segid "BrD " and resid 102  and name HD2%)
  (  segid "BrD " and resid 106  and name HD% )
     3 100     2.400      2 400 peak 28582 weight  0 10000E+01 volume  0 86642E+02 ppm1     1 303 ppm2     7.534
ASSI {28622}
  (  segid "BrD " and resid 102  and name HD2%)
  (( segid "BrD " and resid 28   and name HD2 ))
     3 100     2 400      2 400 peak 28622 weight  0 10000E+01 volume  0 83600E+02 ppm1     1 303 ppm2     5 553
ASSI {28632}
  (  segid "BrD " and resid 102  and name HD2%)
  (( segid "BrD " and resid 106  and name HA  ))
     2 800     2 000      2 000 peak 28632 weight  0.10000E+01 volume  0 15974E+03 ppm1     1 303 ppm2     4 525
ASSI {28642}
  (  segid "BrD " and resid 102  and name HD2%)
  (( segid "BrD " and resid 21   and name HA  ))
     3.500     3 100      2 000 peak 28642 weight  0.10000E+01 volume  0.44750E+02 ppm1     1.303 ppm2     4 354
ASSI {28662}
  (  segid "BrD " and resid 102  and name HD1%)
  (( segid "BrD " and resid 28   and name HD2 ))
     3.200     2 600      2 300 peak 28662 weight  0 10000E+01 volume  0 73306E+02 ppm1     1 303 ppm2     5.574
ASSI {28702}
  (  segid "BrD " and resid 102  and name HD2%)
  (( segid "BrD " and resid 106  and name HB1 ))
     3 600     3 200      1 900 peak 28702 weight  0 10000E+01 volume  0 36289E+02 ppm1     1 303 ppm2     3 882
ASSI {28722}
  (  segid "BrD " and resid 102  and name HD2%)
  (( segid "BrD " and resid 21   and name HB  ))
     3 200     2 600      2 300 peak 28722 weight  0 10000E+01 volume  0 68526E+02 ppm1     1 305 ppm2     2 473
ASSI {28752}
  (  segid "BrD " and resid 102  and name HD2%)
  (  segid "BrD " and resid 78   and name HD2%)
     3 400     2 900      2.100 peak 28752 weight  0 10000E+01 volume  0 55554E+02 ppm1     1.303 ppm2     0 676
ASSI {28782}
  (  segid "BrD " and resid 115  and name HD1%)
  (  segid "BrD " and resid 17   and name HG2%)
     2 200     1 200      1 200 peak 28782 weight  0 10000E+01 volume  0 67664E+03 ppm1     1.352 ppm2     1 750
ASSI {28792}
  (( segid "BrD " and resid 66   and name HG2 ))
  (( segid "BrD " and resid 65   and name HA  ))
     3 000     2 200      2 200 peak 28792 weight  0 10000E+01 volume  0 10599E+03 ppm1     2 141 ppm2     5 395
ASSI {28812}
  (( segid "BrD " and resid 115  and name HB1 ))
  (( segid "BrD " and resid 110  and name HA  ))
     2 400     1 400      1 400 peak 28812 weight  0 10000E+01 volume  0 45932E+03 ppm1     2 190 ppm2     4 419
ASSI {28822}
  (( segid "BrD " and resid 115  and name HG  ))
  (( segid "BrD " and resid 110  and name HA  ))
     2 800     2 000      2 000 peak 28822 weight  0 10000E+01 volume  0 18123E+03 ppm1     2 139 ppm2     4 426
ASSI {28842}
  (( segid "BrD " and resid 115  and name HG  ))
  (  segid "BrD " and resid 110  and name HD1%)
     3.400     2 900      2 100 peak 28842 weight  0 10000E+01 volume  0 47604E+02 ppm1     2.139 ppm2     1 140
ASSI {28852}
  (( segid "BrD " and resid 115  and name HB1 ))
  (  segid "BrD " and resid 113  and name HB% )
     3 600     3 200      1 900 peak 28852 weight  0 10000E+01 volume  0 39467E+02 ppm1     2 190 ppm2     1 978
ASSI {28872}
  (( segid "BrD " and resid 115  and name HB1 ))
  (( segid "BrD " and resid 110  and name HG12))
     2 600     2 600      1 900 peak 28872 weight  0 10000E+01 volume  0 26332E+03 ppm1     2 190 ppm2     1.661
ASSI {28882}
  (( segid "BrD " and resid 115  and name HB1 ))
  (  segid "BrD " and resid 116  and name HD1%)
     2.200     1 200      1 200 peak 28882 weight  0.10000E+01 volume  0 69706E+03 ppm1     2 188 ppm2     1 424
OR {28882}
  (( segid "BrD " and resid 115  and name HB1 ))
  (  segid "BrD " and resid 116  and name HG2%)
ASSI {28892}
  (( segid "BrD " and resid 115  and name HB1 ))
  (( segid "BrD " and resid 116  and name HG12))
     4 000     4 000      1 500 peak 28892 weight  0 10000E+01 volume  0 19745E+02 ppm1     2 188 ppm2     1 583
ASSI {28912}
  (( segid "BrD " and resid 115  and name HA  ))
  (  segid "BrD " and resid 110  and name HG2%)
     3.400     2.900      2 100 peak 28912 weight  0 10000E+01 volume  0 51456E+02 ppm1     4 807 ppm2     1 263
ASSI {28932}
  (  segid "BrD " and resid 56   and name HD1%)
  (( segid "BrD " and resid 35   and name HG1 ))
     3.600     3 200      1 900 peak 28932 weight  0.10000E+01 volume  0 33849E+02 ppm1     1 549 ppm2     3 451
ASSI {28942}
  (  segid "BrD " and resid 56   and name HD1%)
  (( segid "BrD " and resid 35   and name HA  ))
     2.800     2 000      2 000 peak 28942 weight  0 10000E+01 volume  0 16319E+03 ppm1     1 548 ppm2     4 900
ASSI {29012}
  (  segid "BrD " and resid 59   and name HE% )
  (( segid "BrD " and resid 81   and name HB  ))
     2.500     2 500      2 000 peak 29012 weight  0 10000E+01 volume  0.32346E+03 ppm1     1 848 ppm2     2 018
ASSI {29042}
  (  segid "BrD " and resid 59   and name HE% )
  (( segid "BrD " and resid 54   and name HB2 ))
     1 800     1 800      2 700 peak 29042 weight  0 10000E+01 volume  0 22344E+04 ppm1     1 848 ppm2     1 944
ASSI {29052}
  (  segid "BrD " and resid 59   and name HE% )
  (( segid "BrD " and resid 74   and name HB2 ))
     3 900     3 800      1.600 peak 29052 weight  0 10000E+01 volume  0 23714E+02 ppm1     1.848 ppm2     3 002
ASSI {29132}
  (  segid "BrD " and resid 59   and name HE% )
  (( segid "BrD " and resid 77   and name HA  ))
     3 600     3 200      1 900 peak 29132 weight  0 10000E+01 volume  0 36305E+02 ppm1     1 847 ppm2     4 966
ASSI {29142}
  (  segid "BrD " and resid 59   and name HE% )
  (( segid "BrD " and resid 75   and name HA  ))
     4 500     4.500      1 000 peak 29142 weight  0 10000E+01 volume  0 98620E+01 ppm1     1 847 ppm2     4 516
ASSI {29172}
  (  segid "BrD " and resid 54   and name HE% )
  (( segid "BrD " and resid 58   and name HA  ))
     3 500     3 100      2 000 peak 29172 weight  0 10000E+01 volume  0 40557E+02 ppm1     2 536 ppm2     4 468
ASSI {29222}
  (  segid "BrD " and resid 54   and name HE% )
  (( segid "BrD " and resid 57   and name HB2 ))
     2 800     2 000      2.000 peak 29222 weight  0 10000E+01 volume  0 17311E+03 ppm1     2 536 ppm2     2 881
ASSI {29232}
  (  segid "BrD " and resid 54   and name HE% )
  (( segid "BrD " and resid 59   and name HG2 ))
     2 900     2 100      2 100 peak 29232 weight  0 10000E+01 volume  0 12717E+03 ppm1     2 535 ppm2     3 199
OR {29232}
  (  segid "BrD " and resid 54   and name HE% )
  (( segid "BrD " and resid 59   and name HG1 ))
ASSI {29292}
  (( segid "BrD " and resid 54   and name HB2 ))
  (  segid "BrD " and resid 81   and name HG1%)
     3 200     2.600      2 300 peak 29292 weight  0 10000E+01 volume  0 80321E+02 ppm1     1 947 ppm2     1 083
ASSI {29302}
  (  segid "BrD " and resid 54   and name HE% )
  (  segid "BrD " and resid 59   and name HE% )
     3 000     2 200      2.200 peak 29302 weight  0 10000E+01 volume  0 10558E+03 ppm1     2 535 ppm2     1 863
ASSI {29382}
  (( segid "BrD " and resid 33   and name HA  ))
  (( segid "BrD " and resid 32   and name HZ3 ))
     3 200     2 600      2 300 peak 29382 weight  0 10000E+01 volume  0 67859E+02 ppm1     4 361 ppm2     7.811
ASSI {29472}
  (( segid "BrD " and resid 91   and name HG1 ))
  (( segid "BrD " and resid 93   and name HB1 ))
     3 700     3 400      1 800 peak 29472 weight  0 10000E+01 volume  0 32210E+02 ppm1     2 779 ppm2     5 018
OR {29472}
  (( segid "BrD " and resid 91   and name HG1 ))
  (( segid "BrD " and resid 93   and name HA  ))
ASSI {29602}
  (( segid "BrD " and resid 70   and name HA  ))
  (( segid "BrD " and resid 73   and name HB2 ))
     3 600     3 200      1 900 peak 29602 weight  0 10000E+01 volume  0.37115E+02 ppm1     5 346 ppm2     2.483
ASSI {29622}
  (( segid "BrD " and resid 70   and name HB2 ))
  (( segid "BrD " and resid 9    and name HB1 ))
     3 100     2 400      2 400 peak 29622 weight  0 10000E+01 volume  0 85748E+02 ppm1     4 360 ppm2     2 443
ASSI {29632}
  (( segid "BrD " and resid 70   and name HB1 ))
  (( segid "BrD " and resid 9    and name HB1 ))
     3 600     3 200      1.900 peak 29632 weight  0 10000E+01 volume  0 38576E+02 ppm1     4 755 ppm2     2 442
ASSI {29642}
  (( segid "BrD " and resid 93   and name HB2 ))
  (( segid "BrD " and resid 91   and name HD1 ))
     2 300     1 300      1 300 peak 29642 weight  0 10000E+01 volume  0.51818E+03 ppm1     4 755 ppm2     4 550
ASSI {29652}
  (( segid "BrD " and resid 93   and name HB1 ))
  (( segid "BrD " and resid 91   and name HD1 ))
     2 900     2 100      2 100 peak 29652 weight  0 10000E+01 volume  0 14178E+03 ppm1     5 000 ppm2     4 550
ASSI {29662}
  (( segid "BrD " and resid 93   and name HB1 ))
  (( segid "BrD " and resid 94   and name HB1 ))
     3 100     2 400      2 400 peak 29662 weight  0 10000E+01 volume  0 83013E+02 ppm1     5.000 ppm2     2 731
ASSI {29672}
  (( segid "BrD " and resid 93   and name HA  ))
  (( segid "BrD " and resid 91   and name HG1 ))
     3 100     2 400      2 400 peak 29672 weight  0 10000E+01 volume  0 87723E+02 ppm1     5 003 ppm2     2 798
ASSI {29692}
  (( segid "BrD " and resid 108  and name HA  ))
  (( segid "BrD " and resid 111  and name HG2 ))
     4 300     4.300      1 200 peak 29692 weight  0 10000E+01 volume  0 13311E+02 ppm1     4 804 ppm2     1 905
ASSI {29752}
  (( segid "BrD " and resid 30   and name HA  ))
  (  segid "BrD " and resid 102  and name HD1%)
     4.200     4.200      1 300 peak 29752 weight  0.10000E+01 volume  0 14252E+02 ppm1     5 445 ppm2     1 327
ASSI {29772}
  (( segid "BrD " and resid 30   and name HB2 ))
  (( segid "BrD " and resid 28   and name HE1 ))
     3 300     2 700      2 200 peak 29772 weight  0 10000E+01 volume  0 60630E+02 ppm1     4 508 ppm2     8 090
ASSI {29782}
  (( segid "BrD " and resid 30   and name HB2 ))
  (  segid "BrD " and resid 101  and name HG2%)
     3.200     2 600      2 300 peak 29782 weight  0 10000E+01 volume  0 72004E+02 ppm1     4 507 ppm2     1.604
ASSI {29792}
  (( segid "BrD " and resid 27   and name HB1 ))
  (( segid "BrD " and resid 24   and name HB2 ))
     3 400     2 900      2 100 peak 29792 weight  0 10000E+01 volume  0 52302E+02 ppm1     4.607 ppm2     3 077
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OR (29792)
  (( segid "BrD " and resid 27   and name HB1 ))
  (( segid "BrD " and resid 24   and name HG2 ))
ASSI (29832)
  (( segid "BrD " and resid 66   and name HD2 ))
  (( segid "BrD " and resid 65   and name HA  ))
    4 000    4 000     1 500 peak 29832 weight  0.10000E+01 volume  0.19067E+02 ppm1    3 631 ppm2    5 390
ASSI (29842)
  (( segid "BrD " and resid 66   and name HD1 ))
  (( segid "BrD " and resid 65   and name HA  ))
    4 300    4 300     1 200 peak 29842 weight  0 10000E+01 volume  0 12737E+02 ppm1    3 673 ppm2    5 390
ASSI (29852)
  (( segid "BrD " and resid 66   and name HD1 ))
  (  segid "BrD " and resid 15   and name HE% )
    2 800    2 000     2.000 peak 29852 weight  0 10000E+01 volume  0 17551E+03 ppm1    3 673 ppm2    7 488
ASSI (29882)
  (( segid "BrD " and resid 66   and name HD2 ))
  (  segid "BrD " and resid 15   and name HE% )
    2 700    1 800     1 800 peak 29882 weight  0 10000E+01 volume  0 20920E+03 ppm1    3.631 ppm2    7 488
ASSI (29912)
  (( segid "BrD " and resid 66   and name HA  ))
  (( segid "BrD " and resid 65   and name HA  ))
    3.500    3 100     2 000 peak 29912 weight  0 10000E+01 volume  0 40427E+02 ppm1    5 001 ppm2    5 387
ASSI (29922)
  (( segid "BrD " and resid 66   and name HB2 ))
  (( segid "BrD " and resid 65   and name HA  ))
    4 700    4 700     0 800 peak 29922 weight  0 10000E+01 volume  0 75028E+01 ppm1    2 634 ppm2    5 395
ASSI (29982)
  (( segid "BrD " and resid 66   and name HB2 ))
  (  segid "BrD " and resid 69   and name HG1%)
    3 900    3 800     1 600 peak 29982 weight  0.10000E+01 volume  0 23433E+02 ppm1    2 633 ppm2    1 550
ASSI (29992)
  (( segid "BrD " and resid 66   and name HB1 ))
  (  segid "BrD " and resid 69   and name HG1%)
    3 900    3 800     1 600 peak 29992 weight  0 10000E+01 volume  0 22947E+02 ppm1    2 701 ppm2    1 551
ASSI (30022)
  (( segid "BrD " and resid 51   and name HA  ))
  (( segid "BrD " and resid 53   and name HD2 ))
    5 500    5 500     0 000 peak 30022 weight  0 10000E+01 volume  0 72129E-01 ppm1    4 459 ppm2    4.011
ASSI (30062)
  (( segid "BrD " and resid 103  and name HB2 ))
  (( segid "BrD " and resid 82   and name HB1 ))
    3 100    2 400     2 400 peak 30062 weight  0 10000E+01 volume  0 91298E+02 ppm1    1 896 ppm2    3 706
ASSI (30132)
  (( segid "BrD " and resid 116  and name HG11))
  (  segid "BrD " and resid 107  and name HE% )
    2 900    2 100     2 100 peak 30132 weight  0 10000E+01 volume  0 12243E+03 ppm1    1 946 ppm2    7 891
ASSI (30142)
  (( segid "BrD " and resid 116  and name HG11))
  (  segid "BrD " and resid 107  and name HD% )
    3 100    2 400     2 400 peak 30142 weight  0 10000E+01 volume  0 96863E+02 ppm1    1 946 ppm2    7 835
ASSI (30182)
  (( segid "BrD " and resid 64   and name HG1 ))
  (  segid "BrD " and resid 63   and name HD2%)
    3 500    3 100     2 000 peak 30182 weight  0 10000E+01 volume  0 45416E+02 ppm1    2 190 ppm2    1 489
ASSI (30262)
  (( segid "BrD " and resid 86   and name HG1 ))
  (  segid "BrD " and resid 96   and name HD% )
    3 700    3 400     1 800 peak 30262 weight  0 10000E+01 volume  0.30501E+02 ppm1    1 891 ppm2    7 722
ASSI (30322)
  (( segid "BrD " and resid 86   and name HG2 ))
  (( segid "BrD " and resid 87   and name HG1 ))
    3 400    2 900     2 100 peak 30322 weight  0 10000E+01 volume  0 52723E+02 ppm1    0.760 ppm2    3 028
ASSI (30362)
  (( segid "BrD " and resid 103  and name HB2 ))
  (  segid "BrD " and resid 99   and name HB% )
    2.300    1 300     1 300 peak 30362 weight  0 10000E+01 volume  0 49767E+03 ppm1    1 892 ppm2    2.206
ASSI (30422)
  (( segid "BrD " and resid 86   and name HE1 ))
  (  segid "BrD " and resid 99   and name HB% )
    2 500    1 600     1 600 peak 30422 weight  0 10000E+01 volume  0 29716E+03 ppm1    3 078 ppm2    2 206
ASSI (30492)
  (( segid "BrD " and resid 109  and name HE2 ))
  (( segid "BrD " and resid 106  and name HA  ))
    3 000    2 200     2.200 peak 30492 weight  0.10000E+01 volume  0 11843E+03 ppm1    3 029 ppm2    4 591
ASSI (30502)
  (( segid "BrD " and resid 109  and name HE1 ))
  (( segid "BrD " and resid 106  and name HA  ))
    3.800    3 600     1 700 peak 30502 weight  0 10000E+01 volume  0 25593E+02 ppm1    3 177 ppm2    4 590
ASSI (30532)
  (( segid "BrD " and resid 109  and name HD1 ))
  (( segid "BrD " and resid 112  and name HG1 ))
    3.300    2 700     2 200 peak 30532 weight  0 10000E+01 volume  0 67000E+02 ppm1    1 994 ppm2    2 968
ASSI (30682)
  (( segid "BrD " and resid 109  and name HA  ))
  (  segid "BrD " and resid 21   and name HG2%)
    3 600    3 200     1 900 peak 30682 weight  0 10000E+01 volume  0 34166E+02 ppm1    4 656 ppm2    1 588
ASSI (30702)
  (( segid "BrD " and resid 109  and name HA  ))
  (( segid "BrD " and resid 112  and name HG1 ))
    3.800    3 600     1 700 peak 30702 weight  0 10000E+01 volume  0 26014E+02 ppm1    4 653 ppm2    2 964
ASSI (30722)
  (( segid "BrD " and resid 109  and name HA  ))
  (( segid "BrD " and resid 112  and name HG2 ))
    3.200    2.600     2.300 peak 30722 weight  0.10000E+01 volume  0.68767E+02 ppm1    4.653 ppm2    2.823
ASSI (30772)
  (( segid "BrD " and resid 104  and name HB1 ))
  (  segid "BrD " and resid 105  and name HD% )
    3 200    3.600     2 300 peak 30772 weight  0 10000E+01 volume  0.81070E+02 ppm1    2 536 ppm2    7 819
ASSI (30922)
  (( segid "BrD " and resid 19   and name HB1 ))
  (  segid "BrD " and resid 15   and name HE% )
    3 200    2 600     2 300 peak 30922 weight  0.10000E+01 volume  0 75523E+02 ppm1    2 289 ppm2    7 486
ASSI (30962)
  (( segid "BrD " and resid 59   and name HB2 ))
  (( segid "BrD " and resid 56   and name HA  ))
    2 300    1.300     1 300 peak 30962 weight  0 10000E+01 volume  0 51425E+03 ppm1    2 486 ppm2    4 646
ASSI (31062)
  (( segid "BrD " and resid 22   and name HG  ))
  (  segid "BrD " and resid 74   and name HE% )
    2 500    2 500     2 000 peak 31062 weight  0 10000E+01 volume  0.34749E+03 ppm1    2 388 ppm2    7.497
ASSI (31162)
  (( segid "BrD " and resid 54   and name HG1 ))
  (( segid "BrD " and resid 77   and name HA  ))
    3 100    2 400     2 400 peak 31162 weight  0 10000E+01 volume  0 89147E+02 ppm1    3 288 ppm2    4 964
ASSI (   13)
  (  segid "BrD " and resid 46   and name HD% )
  (  segid "BrD " and resid 88   and name HE% )
    2 900    2 100     2 100 peak    13 weight  0 11000E+01 volume  0 62066E+02 ppm1    5 758 ppm2    7 421
ASSI (   23)
  (  segid "BrD " and resid 47   and name HD% )
  (  segid "BrD " and resid 47   and name HE% )
    3 200    2 600     2 300 peak    23 weight  0 11000E+01 volume  0 31210E+02 ppm1    5 758 ppm2    7 261
ASSI (   43)
  (  segid "BrD " and resid 46   and name HE% )
  (  segid "BrD " and resid 88   and name HE% )
    3 800    3 600     1 700 peak    43 weight  0 11000E+01 volume  0 11086E+02 ppm1    6 688 ppm2    7 421
ASSI (   53)
  (  segid "BrD " and resid 46   and name HE% )
  (  segid "BrD " and resid 47   and name HE% )
    4 000    4 000     1 500 peak    53 weight  0 11000E+01 volume  0 78634E+01 ppm1    6 688 ppm2    7 261
ASSI (   93)
  (  segid "BrD " and resid 46   and name HD% )
  (( segid "BrD " and resid 46   and name HA  ))
    2 600    1.700     1 700 peak    93 weight  0 11000E+01 volume  0.11748E+03 ppm1    5.758 ppm2    4 154
ASSI (  103)
  (  segid "BrD " and resid 46   and name HE% )
  (( segid "BrD " and resid 88   and name HB1 ))
    2 300    1 300     1 300 peak   103 weight  0 11000E+01 volume  0 25301E+03 ppm1    6 688 ppm2    3 527
ASSI (  113)
  (  segid "BrD " and resid 46   and name HE% )
  (( segid "BrD " and resid 46   and name HB1 ))
    3 300    2.700     2 200 peak   113 weight  0 11000E+01 volume  0.27341E+02 ppm1    6 688 ppm2    3.279
ASSI (  133)
  (  segid "BrD " and resid 46   and name HD% )
  (( segid "BrD " and resid 46   and name HB2 ))
    2 500    1 600     1 600 peak   133 weight  0 11000E+01 volume  0.14809E+03 ppm1    5 758 ppm2    3.104
ASSI (  153)
  (  segid "BrD " and resid 46   and name HE% )
  (  segid "BrD " and resid 50   and name HD1%)
    3 000    2 200     2 200 peak   153 weight  0 11000E+01 volume  0 42674E+02 ppm1    6 685 ppm2    1 148
ASSI (  273)
  (( segid "BrD " and resid 28   and name HE1 ))
  (( segid "BrD " and resid 28   and name HA  ))
    3 600    3 200     1 900 peak   273 weight  0.11000E+01 volume  0.14248E+02 ppm1    8 129 ppm2    4 533
ASSI (  333)
  (  segid "BrD " and resid 67   and name HD% )
  (  segid "BrD " and resid 68   and name HD% )
    3 000    2 200     2 200 peak   333 weight  0 11000E+01 volume  0 41792E+02 ppm1    6.873 ppm2    7 772
ASSI (  343)
  (  segid "BrD " and resid 67   and name HD% )
  (( segid "BrD " and resid 68   and name HA  ))
    2.800    2 000     2.000 peak   343 weight  0 11000E+01 volume  0 67483E+02 ppm1    6 874 ppm2    5 146
ASSI (  353)
  (  segid "BrD " and resid 67   and name HD% )
  (( segid "BrD " and resid 67   and name HA  ))
    2 500    1 600     1 600 peak   353 weight  0 11000E+01 volume  0 12803E+03 ppm1    6.872 ppm2    4 678
ASSI (  373)
  (  segid "BrD " and resid 67   and name HD% )
  (( segid "BrD " and resid 67   and name HB1 ))
    2 300    1 300     1 300 peak   373 weight  0.11000E+01 volume  0 22980E+03 ppm1    6.874 ppm2    3 570
ASSI (  383)
  (  segid "BrD " and resid 67   and name HE% )
  (  segid "BrD " and resid 68   and name HD% )
    2 900    2 100     2.100 peak   383 weight  0 11000E+01 volume  0.60490E+02 ppm1    7 293 ppm2    7 780
ASSI (  403)
  (  segid "BrD " and resid 67   and name HE% )
  (  segid "BrD " and resid 68   and name HE% )
    2 400    1.400     1.400 peak   403 weight  0.11000E+01 volume  0.16842E+03 ppm1    7.293 ppm2    7.888
ASSI (  433)
  (  segid "BrD " and resid 67   and name HE% )
  (( segid "BrD " and resid 67   and name HA  ))
    3 000    2 200     2 200 peak   433 weight  0 11000E+01 volume  0.50708E+02 ppm1    7 292 ppm2    4 679
ASSI (  463)
  (  segid "BrD " and resid 47   and name HE% )
  (  segid "BrD " and resid 46   and name HD% )
    2 900    2 100     2 100 peak   463 weight  0 11000E+01 volume  0 56184E+02 ppm1    7 246 ppm2    5.744
ASSI (  493)
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  ( segid "BrD " and resid 47   and name HE% )
  (( segid "BrD " and resid 47   and name HA  ))
     3 300     2 700     2 200 peak   493 weight  0 11000E+01 volume  0.27001E+02 ppm1    7 246 ppm2    4 711
ASSI {  503}
  ( segid "BrD " and resid 47   and name HD% )
  (( segid "BrD " and resid 47   and name HA  ))
     2 200     1 200     1 200 peak   503 weight  0 11000E+01 volume  0.29622E+03 ppm1    7 942 ppm2    4.693
ASSI {  543}
  (( segid "BrD " and resid 32   and name HD1 ))
  (( segid "BrD " and resid 30   and name HA  ))
     2 600     1 700     1 700 peak   543 weight  0 11000E+01 volume  0 10449E+03 ppm1    8 455 ppm2    5 452
ASSI {  563}
  (( segid "BrD " and resid 32   and name HD1 ))
  (( segid "BrD " and resid 32   and name HB2 ))
     2 900     2 100     2 100 peak   563 weight  0 11000E+01 volume  0.53265E+02 ppm1    8 456 ppm2    3 942
ASSI {  603}
  ( segid "BrD " and resid 74   and name HD% )
  (( segid "BrD " and resid 74   and name HA  ))
     2 500     1 600     1 600 peak   603 weight  0 11000E+01 volume  0 15470E+03 ppm1    7.013 ppm2    4 373
ASSI {  843}
  ( segid "BrD " and resid 15   and name HD% )
  (( segid "BrD " and resid 15   and name HA  ))
     1 900     0 900     0 900 peak   843 weight  0 11000E+01 volume  0 61725E+03 ppm1    7 664 ppm2    4 621
ASSI {  863}
  ( segid "BrD " and resid 15   and name HD% )
  (( segid "BrD " and resid 15   and name HB1 ))
     2 400     1 400     1 400 peak   863 weight  0 11000E+01 volume  0 19360E+03 ppm1    7 664 ppm2    3 818
ASSI {  873}
  ( segid "BrD " and resid 15   and name HD% )
  (( segid "BrD " and resid 15   and name HB2 ))
     2 000     1 000     1 000 peak   873 weight  0 11000E+01 volume  0 48925E+03 ppm1    7 664 ppm2    3 643
ASSI {  893}
  ( segid "BrD " and resid 15   and name HE% )
  (( segid "BrD " and resid 15   and name HA  ))
     3 500     3 100     2.000 peak   893 weight  0.11000E+01 volume  0 17907E+02 ppm1    7 478 ppm2    4 635
ASSI {  903}
  ( segid "BrD " and resid 15   and name HE% )
  (( segid "BrD " and resid 15   and name HB2 ))
     4 000     4 000     1 500 peak   903 weight  0 11000E+01 volume  0 77515E+01 ppm1    7 478 ppm2    3 643
ASSI {  993}
  ( segid "BrD " and resid 68   and name HE% )
  ( segid "BrD " and resid 74   and name HD% )
     3 100     2 400     2 400 peak   993 weight  0 11000E+01 volume  0 39808E+02 ppm1    7 850 ppm2    6 998
ASSI { 1003}
  ( segid "BrD " and resid 68   and name HE% )
  ( segid "BrD " and resid 67   and name HD% )
     2 900     2 100     2 100 peak  1003 weight  0 11000E+01 volume  0 57511E+02 ppm1    7 850 ppm2    6 896
ASSI { 1063}
  ( segid "BrD " and resid 68   and name HE% )
  (( segid "BrD " and resid 68   and name HA  ))
     2 900     2 100     2 100 peak  1063 weight  0 11000E+01 volume  0 51154E+02 ppm1    7 850 ppm2    5 146
ASSI { 1213}
  ( segid "BrD " and resid 68   and name HD% )
  (( segid "BrD " and resid 68   and name HB1 ))
     2 000     1 000     1 000 peak  1213 weight  0 11000E+01 volume  0 59736E+03 ppm1    7 757 ppm2    3.673
ASSI { 1263}
  ( segid "BrD " and resid 88   and name HD% )
  ( segid "BrD " and resid 46   and name HE% )
     2 800     2.000     2 000 peak  1263 weight  0.11000E+01 volume  0 62764E+02 ppm1    7 618 ppm2    6 692
ASSI { 1283}
  ( segid "BrD " and resid 88   and name HD% )
  ( segid "BrD " and resid 46   and name HD% )
     3 100     2 400     2 400 peak  1283 weight  0 11000E+01 volume  0 38726E+02 ppm1    7 616 ppm2    5 745
ASSI { 1303}
  ( segid "BrD " and resid 88   and name HD% )
  (( segid "BrD " and resid 88   and name HA  ))
     2 200     1 200     1 200 peak  1303 weight  0 11000E+01 volume  0 31179E+03 ppm1    7 616 ppm2    4 999
ASSI { 1313}
  ( segid "BrD " and resid 88   and name HE% )
  (( segid "BrD " and resid 88   and name HA  ))
     2 800     2 000     2 000 peak  1313 weight  0 11000E+01 volume  0 64049E+02 ppm1    7 410 ppm2    4 999
ASSI { 1323}
  ( segid "BrD " and resid 88   and name HD% )
  (( segid "BrD " and resid 46   and name HA  ))
     3 100     2 400     2.400 peak  1323 weight  0 11000E+01 volume  0 38562E+02 ppm1    7 618 ppm2    4 154
ASSI { 1363}
  ( segid "BrD " and resid 88   and name HD% )
  (( segid "BrD " and resid 88   and name HB1 ))
     2 300     1 300     1.300 peak  1363 weight  0 11000E+01 volume  0 21010E+03 ppm1    7 616 ppm2    3.531
ASSI { 1403}
  ( segid "BrD " and resid 96   and name HD% )
  (( segid "BrD " and resid 96   and name HA  ))
     2 400     1 400     1 400 peak  1403 weight  0 11000E+01 volume  0 18299E+03 ppm1    7 711 ppm2    4 431
ASSI { 1413}
  ( segid "BrD " and resid 96   and name HD% )
  (( segid "BrD " and resid 96   and name HB1 ))
     2 400     1 400     1 400 peak  1413 weight  0 11000E+01 volume  0 19687E+03 ppm1    7.712 ppm2    3 996
ASSI { 1503}
  ( segid "BrD " and resid 34   and name HD% )
  (( segid "BrD " and resid 31   and name HA  ))
     2.200     1 200     1 200 peak  1503 weight  0 11000E+01 volume  0 28381E+03 ppm1    7.708 ppm2    4 985
ASSI { 1583}
  ( segid "BrD " and resid 107  and name HE% )
  (( segid "BrD " and resid 107  and name HB1 ))
     3.200     2.600     2.300 peak  1583 weight  0.11000E+01 volume  0.29123E+02 ppm1    7.896 ppm2    3.674
ASSI { 1793}
  ( segid "BrD " and resid 95   and name HD% )
  (( segid "BrD " and resid 95   and name HB2 ))
     3 400     2 900     2.100 peak  1793 weight  0 11000E+01 volume  0 22641E+02 ppm1    7 478 ppm2    3 352
ASSI { 1833}
  ( segid "BrD " and resid 95   and name HD% )
  (( segid "BrD " and resid 95   and name HA  ))
     2 100     1 100     1 100 peak  1833 weight  0 11000E+01 volume  0 35285E+03 ppm1    7 478 ppm2    4 446
ASSI { 1883}
  ( segid "BrD " and resid 95   and name HE% )
  (( segid "BrD " and resid 95   and name HA  ))
     3 400     2 900     2 100 peak  1883 weight  0 11000E+01 volume  0 23591E+02 ppm1    7 617 ppm2    4 446
ASSI { 1943}
  ( segid "BrD " and resid 95   and name HE% )
  (( segid "BrD " and resid 32   and name HH2 ))
     1 800     0 800     0 800 peak  1943 weight  0.11000E+01 volume  0 97461E+03 ppm1    7 619 ppm2    7 785
ASSI { 1963}
  ( segid "BrD " and resid 95   and name HE% )
  (( segid "BrD " and resid 32   and name HZ2 ))
     3 400     2 900     2 100 peak  1963 weight  0 11000E+01 volume  0 21009E+02 ppm1    7 618 ppm2    8 002
ASSI { 2023}
  (( segid "BrD " and resid 32   and name HH2 ))
  (( segid "BrD " and resid 32   and name HZ2 ))
     2 100     1 100     1.100 peak  2023 weight  0 11000E+01 volume  0 40155E+03 ppm1    7 757 ppm2    8 004
ASSI { 2133}
  (( segid "BrD " and resid 82   and name HZ  ))
  ( segid "BrD " and resid 82   and name HD% )
     2 600     1 700     1 700 peak  2133 weight  0 11000E+01 volume  0.10557E+03 ppm1    7 013 ppm2    7 261
ASSI {  163}
  ( segid "BrD " and resid 46   and name HE% )
  ( segid "BrD " and resid 38   and name HG1%)
     3 000     2 200     2 200 peak   163 weight  0 10000E+01 volume  0 48608E+02 ppm1    6 688 ppm2    1 076
ASSI {  183}
  ( segid "BrD " and resid 46   and name HD% )
  (( segid "BrD " and resid 50   and name HB  ))
     3 100     2 400     2 400 peak   183 weight  0 10000E+01 volume  0 36832E+02 ppm1    5 758 ppm2    1 791
ASSI {  253}
  (( segid "BrD " and resid 28   and name HE1 ))
  ( segid "BrD " and resid 101  and name HG2%)
     2 800     2 000     2 000 peak   253 weight  0 10000E+01 volume  0 66486E+02 ppm1    8 130 ppm2    1 601
ASSI {  263}
  (( segid "BrD " and resid 28   and name HE1 ))
  ( segid "BrD " and resid 101  and name HD1%)
     2 600     1 700     1 700 peak   263 weight  0 10000E+01 volume  0 12057E+03 ppm1    8 129 ppm2    1 528
ASSI {  283}
  (( segid "BrD " and resid 28   and name HE1 ))
  (( segid "BrD " and resid 30   and name HB1 ))
     2 900     2 100     2 100 peak   283 weight  0 10000E+01 volume  0.53269E+02 ppm1    8 129 ppm2    4 927
ASSI {  733}
  ( segid "BrD " and resid 74   and name HE% )
  ( segid "BrD " and resid 63   and name HD1%)
     3 700     3 400     1.800 peak   733 weight  0 10000E+01 volume  0 13584E+02 ppm1    7 524 ppm2    1 704
ASSI {  793}
  ( segid "BrD " and resid 82   and name HE% )
  ( segid "BrD " and resid 106  and name HD% )
     3 500     3 100     2 000 peak   793 weight  0 10000E+01 volume  0 18520E+02 ppm1    7 060 ppm2    7 494
ASSI { 1113}
  ( segid "BrD " and resid 68   and name HD% )
  (( segid "BrD " and resid 62   and name HD2 ))
     2.600     1 700     1 700 peak  1113 weight  0 10000E+01 volume  0 11215E+03 ppm1    7 758 ppm2    2 595
ASSI { 1133}
  ( segid "BrD " and resid 68   and name HD% )
  (( segid "BrD " and resid 62   and name HB2 ))
     2 800     2 000     2 000 peak  1133 weight  0 10000E+01 volume  0 66543E+02 ppm1    7 757 ppm2    1 718
ASSI { 1173}
  ( segid "BrD " and resid 105  and name HD% )
  ( segid "BrD " and resid 102  and name HD2%)
     2 800     2 000     2 000 peak  1173 weight  0 10000E+01 volume  0 71257E+02 ppm1    7 758 ppm2    1 338
OR { 1173}
  ( segid "BrD " and resid 105  and name HD% )
  ( segid "BrD " and resid 102  and name HD1%)
ASSI { 1353}
  ( segid "BrD " and resid 88   and name HE% )
  (( segid "BrD " and resid 88   and name HB1 ))
     3 400     2 900     2.100 peak  1353 weight  0 10000E+01 volume  0 21121E+02 ppm1    7 413 ppm2    3 527
ASSI { 1423}
  ( segid "BrD " and resid 96   and name HD% )
  (( segid "BrD " and resid 100  and name HB1 ))
     3.100     2 400     2 400 peak  1423 weight  0 10000E+01 volume  0 40018E+02 ppm1    7 711 ppm2    3 454
OR { 1423}
  ( segid "BrD " and resid 96   and name HD% )
  (( segid "BrD " and resid 100  and name HB2 ))
ASSI { 1613}
  ( segid "BrD " and resid 107  and name HD% )
  (( segid "BrD " and resid 106  and name HB1 ))
     3 600     3 200     1 900 peak  1613 weight  0.10000E+01 volume  0 14818E+02 ppm1    7 803 ppm2    3 953
ASSI { 1663}
  ( segid "BrD " and resid 107  and name HD% )
  (( segid "BrD " and resid 103  and name HA  ))
     3.100     2 400     2 400 peak  1663 weight  0 10000E+01 volume  0.38863E+02 ppm1    7 803 ppm2    3.804
ASSI { 1753}
  ( segid "BrD " and resid 106  and name HE% )
  (( segid "BrD " and resid 75   and name HA  ))
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   3.700      3.400      1.800 peak  1753 weight  0.10000E+01 volume  0.13649E+02 ppm1      7.617 ppm2       4.534
ASSI { 1803}
   ( segid "BrD " and resid 95   and name HD% )
  (( segid "BrD " and resid 85   and name HA  ))
   3.300      2 700      2 200 peak  1803 weight  0 10000E+01 volume  0 27238E+02 ppm1      7 478 ppm2       4 985
ASSI { 1853}
   ( segid "BrD " and resid 95   and name HD% )
  (( segid "BrD " and resid 85   and name HB1 ))
   3 300      2 700      2 200 peak  1853 weight  0 10000E+01 volume  0 27537E+02 ppm1      7.479 ppm2       3 920
ASSI { 1863}
   ( segid "BrD " and resid 95   and name HD% )
  (( segid "BrD " and resid 33   and name HB1 ))
   3.200      2 600      2 300 peak  1863 weight  0 10000E+01 volume  0 30330E+02 ppm1      7 478 ppm2       1 047
ASSI { 1903}
   ( segid "BrD " and resid 95   and name HE% )
  (( segid "BrD " and resid 33   and name HA  ))
   3 500      3 100      2 000 peak  1903 weight  0 10000E+01 volume  0 17985E+02 ppm1      7 618 ppm2       4 343
ASSI { 2003}
  (( segid "BrD " and resid 32   and name HH2 ))
   ( segid "BrD " and resid 95   and name HD% )
   4 300      4 300      1 200 peak  2003 weight  0 10000E+01 volume  0 52192E+01 ppm1      7 757 ppm2       7 509
ASSI { 2143}
  (( segid "BrD " and resid 82   and name HZ  ))
   ( segid "BrD " and resid 106  and name HD% )
   3 800      3 600      1 700 peak  2143 weight  0 10000E+01 volume  0 11127E+02 ppm1      7.013 ppm2       7 509
ASSI { 2183}
   ( segid "BrD " and resid 107  and name HE% )
  (( segid "BrD " and resid 79   and name HG1 ))
   3 500      3 100      2 000 peak  2183 weight  0 10000E+01 volume  0 19805E+02 ppm1      7 897 ppm2       3 060
ASSI {   54}
   ( segid "BrD " and resid 47   and name HD% )
  (( segid "BrD " and resid 47   and name HB1 ))
   2 200      1 200      1 200 peak    54 weight  0 10000E+01 volume  0 95356E+03 ppm1      7 970 ppm2       3 806
ASSI {   64}
   ( segid "BrD " and resid 47   and name HD% )
  (( segid "BrD " and resid 47   and name HB2 ))
   2.300      1 300      1 300 peak    64 weight  0 10000E+01 volume  0 78871E+03 ppm1      7 970 ppm2       3 415
ASSI {  144}
   ( segid "BrD " and resid 67   and name HD% )
   ( segid "BrD " and resid 67   and name HE% )
   2 000      1 000      1 000 peak   144 weight  0 10000E+01 volume  0 18744E+04 ppm1      6 900 ppm2       7 321
ASSI {  214}
   ( segid "BrD " and resid 67   and name HD% )
  (( segid "BrD " and resid 67   and name HB2 ))
   2 200      1 200      1 200 peak   214 weight  0.10000E+01 volume  0 10973E+04 ppm1      6 899 ppm2       2 664
ASSI {  274}
   ( segid "BrD " and resid 68   and name HD% )
  (( segid "BrD " and resid 68   and name HA  ))
   2 400      1 400      1 400 peak   274 weight  0 10000E+01 volume  0 56412E+03 ppm1      7 778 ppm2       5 140
ASSI {  294}
   ( segid "BrD " and resid 68   and name HD% )
  (( segid "BrD " and resid 68   and name HB2 ))
   2 300      1.300      1 300 peak   294 weight  0 10000E+01 volume  0 81340E+03 ppm1      7 778 ppm2       3 546
ASSI {  354}
   ( segid "BrD " and resid 88   and name HD% )
   ( segid "BrD " and resid 88   and name HE% )
   2 000      1 000      1 000 peak   354 weight  0 10000E+01 volume  0 17752E+04 ppm1      7 612 ppm2       7 418
ASSI {  454}
  (( segid "BrD " and resid 32   and name HD1 ))
  (( segid "BrD " and resid 32   and name HA  ))
   3.000      2 200      2 200 peak   454 weight  0 10000E+01 volume  0 17821E+03 ppm1      8 491 ppm2       4.977
ASSI {  474}
  (( segid "BrD " and resid 32   and name HD1 ))
  (( segid "BrD " and resid 32   and name HB1 ))
   3 100      2 400      2 400 peak   474 weight  0 10000E+01 volume  0 14234E+03 ppm1      8 490 ppm2       4 213
ASSI { 1694}
   ( segid "BrD " and resid 34   and name HE% )
  (( segid "BrD " and resid 34   and name HB1 ))
   3 300      2 700      2 200 peak  1694 weight  0 10000E+01 volume  0 91431E+02 ppm1      7 781 ppm2       4 116
ASSI { 1834}
   ( segid "BrD " and resid 96   and name HD% )
   ( segid "BrD " and resid 96   and name HE% )
   1 900      0 900      0 900 peak  1834 weight  0 10000E+01 volume  0 29744E+04 ppm1      7.724 ppm2       7 614
ASSI { 1914}
   ( segid "BrD " and resid 96   and name HD% )
  (( segid "BrD " and resid 96   and name HB2 ))
   2 200      1 200      1 200 peak  1914 weight  0 10000E+01 volume  0 99570E+03 ppm1      7 726 ppm2       3.124
ASSI { 2024}
   ( segid "BrD " and resid 34   and name HD% )
  (( segid "BrD " and resid 34   and name HB1 ))
   2.500      1 600      1 600 peak  2024 weight  0.10000E+01 volume  0 48715E+03 ppm1      7 714 ppm2       4 115
ASSI { 2084}
   ( segid "BrD " and resid 15   and name HD% )
   ( segid "BrD " and resid 15   and name HE% )
   1.900      0 900      0.900 peak  2084 weight  0.10000E+01 volume  0 28924E+04 ppm1      7 689 ppm2       7.483
ASSI { 2474}
   ( segid "BrD " and resid 96   and name HE% )
  (( segid "BrD " and resid 96   and name HB1 ))
   3.300      2 700      2 200 peak  2474 weight  0.10000E+01 volume  0 86809E+02 ppm1      7 611 ppm2       4 001
ASSI { 2554}
   ( segid "BrD " and resid 74   and name HE% )
   ( segid "BrD " and resid 74   and name HD% )
   2 000      1.000      1 000 peak  2554 weight  0.10000E+01 volume  0 18278E+04 ppm1      7 539 ppm2       7 006
ASSI { 3204}
   ( segid "BrD " and resid 82   and name HD% )
  (( segid "BrD " and resid 82   and name HB1 ))
   2 400      1 400      1 400 peak  3204 weight  0 10000E+01 volume  0 67788E+03 ppm1      7 265 ppm2       3 708
ASSI { 3214}
   ( segid "BrD " and resid 82   and name HD% )
  (( segid "BrD " and resid 82   and name HB2 ))
   2 300      1 300      1 300 peak  3214 weight  0 10000E+01 volume  0 77298E+03 ppm1      7 262 ppm2       3 571
ASSI { 3304}
   ( segid "BrD " and resid 82   and name HD% )
   ( segid "BrD " and resid 82   and name HE% )
   2.100      1 100      1 100 peak  3304 weight  0.10000E+01 volume  0.12642E+04 ppm1      7 262 ppm2       7.076
ASSI { 3644}
   ( segid "BrD " and resid 74   and name HD% )
  (( segid "BrD " and resid 74   and name HB2 ))
   2 400      1 400      1 400 peak  3644 weight  0 10000E+01 volume  0 64123E+03 ppm1      7.005 ppm2       3.007
ASSI { 3894}
   ( segid "BrD " and resid 46   and name HD% )
   ( segid "BrD " and resid 46   and name HE% )
   2 000      1 000      1.000 peak  3894 weight  0 10000E+01 volume  0 17599E+04 ppm1      5 743 ppm2       6 687
ASSI { 3914}
   ( segid "BrD " and resid 46   and name HD% )
  (( segid "BrD " and resid 46   and name HB1 ))
   2 400      1 400      1 400 peak  3914 weight  0 10000E+01 volume  0.61947E+03 ppm1      5 740 ppm2       3.304
ASSI { 4064}
  (( segid "BrD " and resid 28   and name HD2 ))
  (( segid "BrD " and resid 28   and name HA  ))
   3 000      2 200      2 200 peak  4064 weight  0 10000E+01 volume  0 15484E+03 ppm1      5.577 ppm2       4 586
ASSI {   84}
   ( segid "BrD " and resid 82   and name HD% )
  (( segid "BrD " and resid 103  and name HA  ))
   2.900      2 100      2 100 peak    84 weight  0 10000E+01 volume  0 22432E+03 ppm1      7 265 ppm2       3 790
ASSI {  174}
   ( segid "BrD " and resid 67   and name HD% )
  (( segid "BrD " and resid 62   and name HA  ))
   3 300      2 700      2 200 peak   174 weight  0.10000E+01 volume  0 89209E+02 ppm1      6 899 ppm2       4 490
ASSI {  244}
   ( segid "BrD " and resid 67   and name HD% )
  (( segid "BrD " and resid 62   and name HB2 ))
   2 900      2.100      2 100 peak   244 weight  0 10000E+01 volume  0 21286E+03 ppm1      6 899 ppm2       1 706
ASSI {  254}
   ( segid "BrD " and resid 67   and name HD% )
   ( segid "BrD " and resid 73   and name HD1%)
   3.500      3 100      2 000 peak   254 weight  0 10000E+01 volume  0 64742E+02 ppm1      6.899 ppm2       1.545
ASSI {  464}
  (( segid "BrD " and resid 32   and name HD1 ))
  (( segid "BrD " and resid 29   and name HA  ))
   3 300      2 700      2 200 peak   464 weight  0 10000E+01 volume  0 97341E+02 ppm1      8 490 ppm2       4 814
ASSI {  494}
  (( segid "BrD " and resid 32   and name HD1 ))
  (( segid "BrD " and resid 33   and name HD1 ))
   5.500      5 500      0 000 peak   494 weight  0 10000E+01 volume  0 38880E-03 ppm1      8 490 ppm2       2 781
ASSI {  504}
  (( segid "BrD " and resid 32   and name HD1 ))
  (( segid "BrD " and resid 33   and name HD2 ))
   4 000      4 000      1.500 peak   504 weight  0 10000E+01 volume  0 30117E+02 ppm1      8 490 ppm2       2 211
ASSI {  564}
  (( segid "BrD " and resid 107  and name HZ  ))
  (( segid "BrD " and resid 79   and name HB1 ))
   3.100      2 400      2 400 peak   564 weight  0 10000E+01 volume  0 14239E+03 ppm1      8 008 ppm2       2 802
ASSI {  624}
  (( segid "BrD " and resid 107  and name HZ  ))
  (( segid "BrD " and resid 79   and name HA  ))
   3.000      2 200      2 200 peak   624 weight  0 10000E+01 volume  0 17938E+03 ppm1      8 058 ppm2       4 439
ASSI {  634}
  (( segid "BrD " and resid 107  and name HZ  ))
   ( segid "BrD " and resid 107  and name HE% )
   2 000      1 000      1.000 peak   634 weight  0 10000E+01 volume  0 19583E+04 ppm1      8 058 ppm2       7 927
ASSI {  644}
  (( segid "BrD " and resid 107  and name HZ  ))
   ( segid "BrD " and resid 107  and name HD% )
   2.500      2.500      2 000 peak   644 weight  0 10000E+01 volume  0.49678E+03 ppm1      8 058 ppm2       7 793
ASSI {  664}
  (( segid "BrD " and resid 107  and name HZ  ))
  (( segid "BrD " and resid 79   and name HG1 ))
   2 700      1.800      1 800 peak   664 weight  0 10000E+01 volume  0 34018E+03 ppm1      8 059 ppm2       2 994
ASSI {  694}
  (( segid "BrD " and resid 32   and name HZ2 ))
  (( segid "BrD " and resid 94   and name HG1 ))
   2 500      1 600      1 600 peak   694 weight  0 10000E+01 volume  0.45123E+03 ppm1      8 008 ppm2       3 154
ASSI {  714}
  (( segid "BrD " and resid 32   and name HZ2 ))
  (( segid "BrD " and resid 32   and name HZ3 ))
   2 100      2.100      2 400 peak   714 weight  0 10000E+01 volume  0 13157E+04 ppm1      8 004 ppm2       7.797
ASSI {  724}
  (( segid "BrD " and resid 32   and name HE3 ))
  (( segid "BrD " and resid 33   and name HG2 ))
   3.200      2.600      2 300 peak   724 weight  0 10000E+01 volume  0.11962E+03 ppm1      7 959 ppm2      -0 311
ASSI {  804}
  (( segid "BrD " and resid 32   and name HZ2 ))
  (( segid "BrD " and resid 97   and name HB1 ))
   2.700      1.800      1 800 peak   804 weight  0.10000E+01 volume  0.29399E+03 ppm1      7 961 ppm2       2 667
ASSI {  854}
  (( segid "BrD " and resid 32   and name HE3 ))
  (( segid "BrD " and resid 32   and name HA  ))
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   2.900     2.100     2.100 peak   854 weight  0.10000E+01 volume  0.19220E+03 ppm1     7.957 ppm2     4.976
ASSI {  864}
  (( segid "BrD " and resid 32    and name HE3 ))
  (( segid "BrD " and resid 33    and name HA  ))
   2 600     1 700     1.700 peak   864 weight  0.10000E+01 volume  0 35337E+03 ppm1     7 956 ppm2     4.361
ASSI {  874}
  (( segid "BrD " and resid 32    and name HE3 ))
  (( segid "BrD " and resid 32    and name HB1 ))
   2 800     2 000     2 000 peak   874 weight  0 10000E+01 volume  0 24249E+03 ppm1     7 958 ppm2     3 966
ASSI {  984}
  (  segid "BrD " and resid 107   and name HE% )
  (( segid "BrD " and resid 103   and name HA  ))
   3 000     2 200     2 200 peak   984 weight  0 10000E+01 volume  0 17386E+03 ppm1     7 925 ppm2     3 742
ASSI { 1024}
  (( segid "BrD " and resid 34    and name HZ  ))
  (( segid "BrD " and resid 102   and name HB2 ))
   2 500     1 600     1.600 peak  1024 weight  0.10000E+01 volume  0 46463E+03 ppm1     7 926 ppm2     1.813
ASSI { 1144}
  (( segid "BrD " and resid 34    and name HZ  ))
  (( segid "BrD " and resid 102   and name HB1 ))
   2 900     2 100     2 100 peak  1144 weight  0 10000E+01 volume  0 21471E+03 ppm1     7 900 ppm2     1 967
ASSI { 1154}
  (( segid "BrD " and resid 34    and name HZ  ))
  (( segid "BrD " and resid 98    and name HB1 ))
   3 300     2 700     2 200 peak  1154 weight  0.10000E+01 volume  0 95962E+02 ppm1     7.899 ppm2     4 001
ASSI { 1194}
  (  segid "BrD " and resid 107   and name HE% )
  (( segid "BrD " and resid 79    and name HA  ))
   2 300     1 300     1 300 peak  1194 weight  0 10000E+01 volume  0 84240E+03 ppm1     7 889 ppm2     4 391
ASSI { 1224}
  (  segid "BrD " and resid 68    and name HE% )
  (( segid "BrD " and resid 62    and name HD1 ))
   3 100     2 400     2.400 peak  1224 weight  0 10000E+01 volume  0 13020E+03 ppm1     7 892 ppm2     3 172
ASSI { 1314}
  (  segid "BrD " and resid 68    and name HE% )
  (  segid "BrD " and resid 73    and name HD2%)
   4 100     4 100     1 400 peak  1314 weight  0 10000E+01 volume  0 23932E+02 ppm1     7 892 ppm2     1 496
ASSI { 1344}
  (( segid "BrD " and resid 32    and name HE3 ))
  (( segid "BrD " and resid 33    and name HD2 ))
   3 200     2 600     2 300 peak  1344 weight  0 10000E+01 volume  0 10782E+03 ppm1     7 956 ppm2     2 212
ASSI { 1434}
  (( segid "BrD " and resid 32    and name HZ3 ))
  (( segid "BrD " and resid 32    and name HE3 ))
   1 800     0 800     0 800 peak  1434 weight  0 10000E+01 volume  0 39856E+04 ppm1     7 812 ppm2     7 954
ASSI { 1454}
  (  segid "BrD " and resid 34    and name HE% )
  (  segid "BrD " and resid 102   and name HD1%)
   2 900     2 100     2 100 peak  1454 weight  0 10000E+01 volume  0 19468E+03 ppm1     7 808 ppm2     1 268
ASSI { 1464}
  (  segid "BrD " and resid 107   and name HD% )
  (  segid "BrD " and resid 110   and name HD1%)
   2 800     2 000     2 000 peak  1464 weight  0 10000E+01 volume  0 23444E+03 ppm1     7.810 ppm2     1 153
ASSI { 1474}
  (  segid "BrD " and resid 107   and name HD% )
  (  segid "BrD " and resid 116   and name HD1%)
   2 600     1 700     1 700 peak  1474 weight  0.10000E+01 volume  0 36349E+03 ppm1     7 806 ppm2     1 399
ASSI { 1494}
  (  segid "BrD " and resid 107   and name HD% )
  (( segid "BrD " and resid 107   and name HA  ))
   2.300     1 300     1 300 peak  1494 weight  0 10000E+01 volume  0 85611E+03 ppm1     7 803 ppm2     4 440
ASSI { 1524}
  (  segid "BrD " and resid 105   and name HD% )
  (( segid "BrD " and resid 105   and name HB1 ))
   2 300     1 300     1 300 peak  1524 weight  0 10000E+01 volume  0 86322E+03 ppm1     7 798 ppm2     3 741
ASSI { 1564}
  (  segid "BrD " and resid 34    and name HE% )
  (( segid "BrD " and resid 28    and name HD2 ))
   3 000     2 200     2.200 peak  1564 weight  0 10000E+01 volume  0 16881E+03 ppm1     7 794 ppm2     5 562
ASSI { 1594}
  (( segid "BrD " and resid 32    and name HZ3 ))
  (  segid "BrD " and resid 95    and name HE% )
   2.600     1 700     1 700 peak  1594 weight  0.10000E+01 volume  0 36507E+03 ppm1     7 791 ppm2     7 630
ASSI { 1634}
  (  segid "BrD " and resid 34    and name HE% )
  (( segid "BrD " and resid 102   and name HB1 ))
   3 200     2 600     2.300 peak  1634 weight  0 10000E+01 volume  0 12088E+03 ppm1     7 790 ppm2     2 032
ASSI { 1644}
  (  segid "BrD " and resid 34    and name HE% )
  (( segid "BrD " and resid 98    and name HB1 ))
   2 700     1 800     1 800 peak  1644 weight  0 10000E+01 volume  0 32157E+03 ppm1     7 784 ppm2     4 016
ASSI { 1724}
  (  segid "BrD " and resid 107   and name HD% )
  (( segid "BrD " and resid 103   and name HG2 ))
   2 400     2 400     2.100 peak  1724 weight  0 10000E+01 volume  0 57448E+03 ppm1     7 778 ppm2     2 487
ASSI { 1754}
  (( segid "BrD " and resid 32    and name HZ3 ))
  (( segid "BrD " and resid 33    and name HB1 ))
   2.700     1 800     1 800 peak  1754 weight  0.10000E+01 volume  0 30103E+03 ppm1     7 780 ppm2     1 088
ASSI { 1764}
  (  segid "BrD " and resid 34    and name HE% )
  (  segid "BrD " and resid 81    and name HG2%)
   3 000     2.200     2.200 peak  1764 weight  0.10000E+01 volume  0 16442E+03 ppm1     7 781 ppm2     0 762
ASSI { 1794}
  (  segid "BrD " and resid 68    and name HD% )
  (  segid "BrD " and resid 73    and name HD1%)
   2 600     1.700     1.700 peak  1794 weight  0 10000E+01 volume  0 42209E+03 ppm1     7 781 ppm2     1 543
ASSI { 1904}
  (  segid "BrD " and resid 34    and name HD% )
  (( segid "BrD " and resid 34    and name HZ  ))
   2 600     1 700     1 700 peak  1904 weight  0 10000E+01 volume  0 35620E+03 ppm1     7.719 ppm2     7 901
ASSI { 1954}
  (  segid "BrD " and resid 34    and name HD% )
  (( segid "BrD " and resid 85    and name HB1 ))
   3 000     2 200     2 200 peak  1954 weight  0 10000E+01 volume  0 18188E+03 ppm1     7 714 ppm2     3 920
ASSI { 2124}
  (  segid "BrD " and resid 15    and name HD% )
  (  segid "BrD " and resid 63    and name HD1%)
   2.500     1.600     1 600 peak  2124 weight  0 10000E+01 volume  0 44171E+03 ppm1     7 689 ppm2     1 641
ASSI { 2164}
  (  segid "BrD " and resid 15    and name HD% )
  (( segid "BrD " and resid 16    and name HA  ))
   2.600     1 700     1 700 peak  2164 weight  0 10000E+01 volume  0 41516E+03 ppm1     7 650 ppm2     4 538
ASSI { 2224}
  (  segid "BrD " and resid 106   and name HE% )
  (  segid "BrD " and resid 75    and name HE% )
   3 000     2.200     2 200 peak  2224 weight  0 10000E+01 volume  0 17361E+03 ppm1     7 646 ppm2     2 666
ASSI { 2234}
  (  segid "BrD " and resid 106   and name HE% )
  (( segid "BrD " and resid 78    and name HB1 ))
   2 900     2 100     2 100 peak  2234 weight  0 10000E+01 volume  0 21480E+03 ppm1     7 647 ppm2     1 333
ASSI { 2244}
  (  segid "BrD " and resid 106   and name HE% )
  (( segid "BrD " and resid 78    and name HB1 ))
   2 600     1 700     1 700 peak  2244 weight  0 10000E+01 volume  0 42175E+03 ppm1     7 647 ppm2     1 268
OR { 2244}
  (  segid "BrD " and resid 106   and name HE% )
  (( segid "BrD " and resid 78    and name HG  ))
ASSI { 2264}
  (  segid "BrD " and resid 106   and name HE% )
  (( segid "BrD " and resid 106   and name HB1 ))
   3 400     2 900     2 100 peak  2264 weight  0 10000E+01 volume  0 80420E+02 ppm1     7 644 ppm2     3 919
ASSI { 2414}
  (  segid "BrD " and resid 106   and name HE% )
  (  segid "BrD " and resid 17    and name HG2%)
   4 000     4 000     1 500 peak  2414 weight  0.10000E+01 volume  0 29483E+02 ppm1     7 616 ppm2     1 706
ASSI { 2484}
  (  segid "BrD " and resid 96    and name HE% )
  (( segid "BrD " and resid 86    and name HE1 ))
   3 000     2 200     2 200 peak  2484 weight  0 10000E+01 volume  0 16268E+03 ppm1     7 611 ppm2     3 106
ASSI { 2504}
  (  segid "BrD " and resid 106   and name HE% )
  (( segid "BrD " and resid 21    and name HG11))
   2.500     1 600     1 600 peak  2504 weight  0 10000E+01 volume  0 54543E+03 ppm1     7 611 ppm2     2 374
ASSI { 2514}
  (  segid "BrD " and resid 106   and name HE% )
  (( segid "BrD " and resid 18    and name HG  ))
   2 600     1 700     1 700 peak  2514 weight  0 10000E+01 volume  0 40048E+03 ppm1     7 611 ppm2     2 274
ASSI { 2574}
  (  segid "BrD " and resid 74    and name HE% )
  (  segid "BrD " and resid 63    and name HD2%)
   2 900     2 100     2 100 peak  2574 weight  0 10000E+01 volume  0 18991E+03 ppm1     7 539 ppm2     1 496
ASSI { 2614}
  (  segid "BrD " and resid 106   and name HD% )
  (( segid "BrD " and resid 21    and name HG11))
   3 200     2 600     2 300 peak  2614 weight  0 10000E+01 volume  0 10679E+03 ppm1     7 535 ppm2     2 308
ASSI { 2654}
  (  segid "BrD " and resid 106   and name HD% )
  (  segid "BrD " and resid 21    and name HG2%)
   2 000     1.000     1.000 peak  2654 weight  0.10000E+01 volume  0 21819E+04 ppm1     7.541 ppm2     1 580
ASSI { 2674}
  (  segid "BrD " and resid 74    and name HE% )
  (( segid "BrD " and resid 78    and name HG  ))
   2 500     1.600     1 600 peak  2674 weight  0 10000E+01 volume  0 54850E+03 ppm1     7 529 ppm2     1 266
ASSI { 2694}
  (  segid "BrD " and resid 74    and name HE% )
  (  segid "BrD " and resid 78    and name HD1%)
   2.500     1 600     1 600 peak  2694 weight  0 10000E+01 volume  0 46858E+03 ppm1     7 530 ppm2     0 780
ASSI { 2754}
  (  segid "BrD " and resid 106   and name HD% )
  (( segid "BrD " and resid 106   and name HB1 ))
   2 300     1.300     1 300 peak  2754 weight  0 10000E+01 volume  0 86816E+03 ppm1     7.524 ppm2     3 919
ASSI { 2774}
  (  segid "BrD " and resid 106   and name HD% )
  (( segid "BrD " and resid 106   and name HB2 ))
   2 400     1.400     1 400 peak  2774 weight  0 10000E+01 volume  0 63063E+03 ppm1     7.524 ppm2     3 708
ASSI { 2834}
  (  segid "BrD " and resid 106   and name HD% )
  (  segid "BrD " and resid 107   and name HE% )
   3 400     2 900     2 100 peak  2834 weight  0 10000E+01 volume  0 82229E+02 ppm1     7 513 ppm2     7 940
ASSI { 3074}
  (  segid "BrD " and resid 67    and name HE% )
  (  segid "BrD " and resid 73    and name HD1%)
   4 000     4 000     1 500 peak  3074 weight  0 10000E+01 volume  0 28072E+02 ppm1     7 318 ppm2     1 545
ASSI { 3144}
  (  segid "BrD " and resid 47    and name HE% )
  (( segid "BrD " and resid 46    and name HB2 ))
   3 000     2.200     2 200 peak  3144 weight  0 10000E+01 volume  0 17782E+03 ppm1     7 270 ppm2     3.075
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ASSI { 3224}
  ( segid "BrD " and resid 82   and name HD% )
  (( segid "BrD " and resid 103  and name HG1 ))
    3.100     2 400     2 400 peak  3224 weight  0.10000E+01 volume  0 12400E+03 ppm1     7 264 ppm2     2 595
ASSI { 3234}
  ( segid "BrD " and resid 82   and name HD% )
  (( segid "BrD " and resid 103  and name HB1 ))
    3 200     2 600     2 300 peak  3234 weight  0 10000E+01 volume  0 10914E+03 ppm1     7.266 ppm2     2 374
ASSI { 3254}
  ( segid "BrD " and resid 82   and name HD% )
  (( segid "BrD " and resid 81   and name HB  ))
    3.200     2 600     2 300 peak  3254 weight  0 10000E+01 volume  0 12188E+03 ppm1     7 266 ppm2     2 032
ASSI { 3264}
  ( segid "BrD " and resid 82   and name HD% )
  (( segid "BrD " and resid 103  and name HB2 ))
    3 100     2 400     2 400 peak  3264 weight  0 10000E+01 volume  0 13715E+03 ppm1     7 266 ppm2     1 902
ASSI { 3314}
  ( segid "BrD " and resid 82   and name HD% )
  ( segid "BrD " and resid 102  and name HD2%)
    3 100     2 400     2 400 peak  3314 weight  0 10000E+01 volume  0 13023E+03 ppm1     7 261 ppm2     1.332
OR { 3314}
  ( segid "BrD " and resid 82   and name HD% )
  ( segid "BrD " and resid 102  and name HD1%)
ASSI { 3354}
  ( segid "BrD " and resid 82   and name HE% )
  (( segid "BrD " and resid 106  and name HB1 ))
    3 000     2 200     2 200 peak  3354 weight  0 10000E+01 volume  0 15234E+03 ppm1     7 069 ppm2     3 922
ASSI { 3364}
  ( segid "BrD " and resid 82   and name HE% )
  (( segid "BrD " and resid 103  and name HA  ))
    3 000     2 200     2 200 peak  3364 weight  0.10000E+01 volume  0 15995E+03 ppm1     7.070 ppm2     3 789
ASSI { 3404}
  ( segid "BrD " and resid 82   and name HE% )
  (( segid "BrD " and resid 102  and name HB2 ))
    2 900     2 100     2 100 peak  3404 weight  0 10000E+01 volume  0 20703E+03 ppm1     7 070 ppm2     1 838
ASSI { 3424}
  ( segid "BrD " and resid 82   and name HE% )
  ( segid "BrD " and resid 102  and name HD2%)
    2 400     1 400     1 400 peak  3424 weight  0 10000E+01 volume  0 67243E+03 ppm1     7 070 ppm2     1.333
ASSI { 3444}
  ( segid "BrD " and resid 82   and name HE% )
  ( segid "BrD " and resid 107  and name HD% )
    3 500     3 100     2 000 peak  3444 weight  0 10000E+01 volume  0 65231E+02 ppm1     7.069 ppm2     7 777
ASSI { 3464}
  ( segid "BrD " and resid 82   and name HE% )
  ( segid "BrD " and resid 78   and name HD2%)
    2 900     2 100     2 100 peak  3464 weight  0.10000E+01 volume  0 20065E+03 ppm1     7 067 ppm2     0 680
ASSI { 3514}
  (( segid "BrD " and resid 82   and name HZ  ))
  ( segid "BrD " and resid 102  and name HD2%)
    3 200     2 600     2 300 peak  3514 weight  0 10000E+01 volume  0 11748E+03 ppm1     7 021 ppm2     1 331
ASSI { 3524}
  (( segid "BrD " and resid 82   and name HZ  ))
  ( segid "BrD " and resid 78   and name HD2%)
    2 800     2 000     2 000 peak  3524 weight  0.10000E+01 volume  0 25407E+03 ppm1     7 017 ppm2     0 681
ASSI { 3574}
  ( segid "BrD " and resid 74   and name HD% )
  ( segid "BrD " and resid 68   and name HD% )
    2 800     2 000     2 000 peak  3574 weight  0 10000E+01 volume  0 24279E+03 ppm1     7 005 ppm2     7 777
ASSI { 3654}
  ( segid "BrD " and resid 74   and name HD% )
  ( segid "BrD " and resid 75   and name HE% )
    3 300     2.700     2.200 peak  3654 weight  0 10000E+01 volume  0 90985E+02 ppm1     7 005 ppm2     2.667
ASSI { 3684}
  ( segid "BrD " and resid 74   and name HD% )
  ( segid "BrD " and resid 59   and name HE% )
    2 600     1 700     1.700 peak  3684 weight  0 10000E+01 volume  0.36097E+03 ppm1     7 005 ppm2     1.885
ASSI { 3754}
  ( segid "BrD " and resid 67   and name HD% )
  (( segid "BrD " and resid 62   and name HG2 ))
    3 400     2 900     2 100 peak  3754 weight  0 10000E+01 volume  0 78199E+02 ppm1     6 899 ppm2     1 496
ASSI { 3804}
  ( segid "BrD " and resid 46   and name HE% )
  (( segid "BrD " and resid 53   and name HA  ))
    3 100     2.400     2 400 peak  3804 weight  0 10000E+01 volume  0 13088E+03 ppm1     6 686 ppm2     4 701
ASSI { 3944}
  ( segid "BrD " and resid 46   and name HD% )
  ( segid "BrD " and resid 38   and name HG1%)
    3 400     2 900     2.100 peak  3944 weight  0 10000E+01 volume  0 75575E+02 ppm1     5 740 ppm2     1 088
ASSI { 4024}
  (( segid "BrD " and resid 52   and name HA  ))
  (( segid "BrD " and resid 53   and name HD2 ))
    3.400     2.900     2 100 peak  4024 weight  0.10000E+01 volume  0 78758E+02 ppm1     5 589 ppm2     4 017
ASSI { 4054}
  (( segid "BrD " and resid 28   and name HD2 ))
  (( segid "BrD " and resid 34   and name HZ  ))
    2.800     2 000     2 000 peak  4054 weight  0 10000E+01 volume  0 24761E+03 ppm1     5 577 ppm2     7 924
ASSI { 4114}
  (( segid "BrD " and resid 34   and name HA  ))
  ( segid "BrD " and resid 34   and name HD% )
    2 300     1.300     1.300 peak  4114 weight  0 10000E+01 volume  0 78719E+03 ppm1     5 547 ppm2     7 713
ASSI { 4204}
  ( segid "BrD " and resid 34   and name HD% )
  ( segid "BrD " and resid 56   and name HD1%)
    2.900     2.100     2.100 peak  4204 weight  0.10000E+01 volume  0.22356E+03 ppm1     7.714 ppm2     1.544
ASSI { 4264}
  ( segid "BrD " and resid 34   and name HE% )
  (( segid "BrD " and resid 31   and name HA  ))
    2.500     1 600     1 600 peak  4264 weight  0 10000E+01 volume  0 48557E+03 ppm1     7 781 ppm2     4 993
ASSI { 4304}
  ( segid "BrD " and resid 107  and name HD% )
  ( segid "BrD " and resid 106  and name HD% )
    2 800     2 000     2.000 peak  4304 weight  0 10000E+01 volume  0 27783E+03 ppm1     7 802 ppm2     7 517
ASSI { 4324}
  (( segid "BrD " and resid 82   and name HZ  ))
  (( segid "BrD " and resid 103  and name HA  ))
    3.300     2 700     2 200 peak  4324 weight  0.10000E+01 volume  0 96267E+02 ppm1     7 031 ppm2     3 790
ASSI { 4364}
  ( segid "BrD " and resid 107  and name HE% )
  (( segid "BrD " and resid 78   and name HB2 ))
    3 400     2 900     2 100 peak  4364 weight  0.10000E+01 volume  0 78224E+02 ppm1     7 888 ppm2     1 085
ASSI {    5}
  (( segid "AcH " and resid 201  and name HA1 ))
  ( segid "BrD " and resid 38   and name HG1%)
    2.600     1 700     1 700 peak     5 weight  0.11000E+01 volume  0 16527E+03 ppm1     4 029 ppm2     1 081
OR {    5}
  (( segid "AcH " and resid 201  and name HA2 ))
  ( segid "BrD " and resid 38   and name HG1%)
ASSI {   15}
  (( segid "AcH " and resid 201  and name HA1 ))
  ( segid "BrD " and resid 38   and name HG2%)
    2.600     1 700     1 700 peak    15 weight  0 11000E+01 volume  0 14933E+03 ppm1     4 026 ppm2     0 723
OR {   15}
  (( segid "AcH " and resid 201  and name HA2 ))
  ( segid "BrD " and resid 38   and name HG2%)
ASSI {   25}
  (( segid "AcH " and resid 201  and name HA1 ))
  ( segid "BrD " and resid 43   and name HB% )
    2 600     1 700     1 700 peak    25 weight  0 11000E+01 volume  0 16374E+03 ppm1     4.023 ppm2     1 609
ASSI {   35}
  (( segid "AcH " and resid 201  and name HB2 ))
  ( segid "BrD " and resid 43   and name HB% )
    2.600     1 700     1 700 peak    35 weight  0.11000E+01 volume  0 16831E+03 ppm1     3 428 ppm2     1 601
ASSI {   45}
  (( segid "AcH " and resid 201  and name HB2 ))
  ( segid "BrD " and resid 38   and name HG1%)
    2 700     1 800     1 800 peak    45 weight  0 11000E+01 volume  0 14392E+03 ppm1     3 430 ppm2     1 074
OR {   45}
  (( segid "AcH " and resid 201  and name HB1 ))
  ( segid "BrD " and resid 38   and name HG1%)
ASSI {   55}
  (( segid "AcH " and resid 201  and name HB2 ))
  ( segid "BrD " and resid 38   and name HG2%)
    2.600     1 700     1 700 peak    55 weight  0 11000E+01 volume  0 14742E+03 ppm1     3 430 ppm2     0 723
OR {   55}
  (( segid "AcH " and resid 201  and name HB1 ))
  ( segid "BrD " and resid 38   and name HG2%)
ASSI {   65}
  (( segid "AcH " and resid 201  and name HD1 ))
  ( segid "BrD " and resid 43   and name HB% )
    2.600     1.700     1 700 peak    65 weight  0 11000E+01 volume  0 15413E+03 ppm1     8 179 ppm2     1 608
ASSI {   75}
  (( segid "AcH " and resid 201  and name HD2 ))
  ( segid "BrD " and resid 43   and name HB% )
    2 700     1 800     1 800 peak    75 weight  0 11000E+01 volume  0 13471E+03 ppm1     7 683 ppm2     1 592
ASSI {   85}
  (( segid "AcH " and resid 201  and name HD2 ))
  ( segid "BrD " and resid 38   and name HG1%)
    2.700     1 800     1 800 peak    85 weight  0 11000E+01 volume  0 12532E+03 ppm1     7 680 ppm2     1 066
ASSI {   95}
  (( segid "AcH " and resid 201  and name HD2 ))
  ( segid "BrD " and resid 38   and name HG2%)
    2 700     1 800     1 800 peak    95 weight  0 11000E+01 volume  0 12585E+03 ppm1     7 690 ppm2     0.691
ASSI {  105}
  ( segid "AcH " and resid 200  and name HA% )
  ( segid "BrD " and resid 38   and name HG2%)
    2 600     1 700     1.700 peak   105 weight  0.11000E+01 volume  0 16395E+03 ppm1     2 547 ppm2     0 727
ASSI {  115}
  ( segid "AcH " and resid 200  and name HA% )
  ( segid "BrD " and resid 38   and name HG1%)
    2 400     1 400     1 400 peak   115 weight  0 11000E+01 volume  0 29029E+03 ppm1     2 548 ppm2     1.072
ASSI {  125}
  ( segid "AcH " and resid 200  and name HA% )
  ( segid "BrD " and resid 43   and name HB% )
    2.700     1.800     1 800 peak   125 weight  0 11000E+01 volume  0 13320E+03 ppm1     2 538 ppm2     1 603
ASSI {  135}
  ( segid "AcH " and resid 200  and name HA% )
  (( segid "BrD " and resid 38   and name HA  ))
    2.600     1.700     1 700 peak   135 weight  0.11000E+01 volume  0 17326E+03 ppm1     2 548 ppm2     4 209
ASSI {  145}
  ( segid "AcH " and resid 200  and name HA% )
  (( segid "BrD " and resid 43   and name HA  ))
    2 700     1 800     1 800 peak   145 weight  0 11000E+01 volume  0 12382E+03 ppm1     2 547 ppm2     5 520
ASSI {    6}
  (( segid "AcH " and resid 201  and name HA1 ))
  ( segid "BrD " and resid 46   and name HE% )
    2 700     1 800     1 800 peak     6 weight  0 11000E+01 volume  0 14312E+03 ppm1     4.007 ppm2     6.648
OR {    6}
```

```
  (( segid "AcH " and resid 201  and name HA2 ))
  (  segid "BrD " and resid 46   and name HE% )
ASSI {   16}
  (( segid "AcH " and resid 201  and name HA2 ))
  (  segid "BrD " and resid 95   and name HD% )
    2 700      1 800      1 800 peak     16 weight  0 11000E+01 volume  0.13924E+03 ppm1      4.015 ppm2      7 481
OR {   16}
  (( segid "AcH " and resid 201  and name HA1 ))
  (  segid "BrD " and resid 95   and name HD% )
ASSI {   26}
  (( segid "AcH " and resid 201  and name HB1 ))
  (  segid "BrD " and resid 95   and name HD% )
    2.600      1 700      1 700 peak     26 weight  0.11000E+01 volume  0.15229E+03 ppm1      3.429 ppm2      7 481
OR {   26}
  (( segid "AcH " and resid 201  and name HB2 ))
  (  segid "BrD " and resid 95   and name HD% )
ASSI {   36}
  (( segid "AcH " and resid 201  and name HA1 ))
  (  segid "BrD " and resid 88   and name HD% )
    2.500      1 600      1 600 peak     36 weight  0.11000E+01 volume  0 18465E+03 ppm1      4.015 ppm2      7 637
OR {   36}
  (( segid "AcH " and resid 201  and name HA2 ))
  (  segid "BrD " and resid 88   and name HD% )
ASSI {   46}
  (( segid "AcH " and resid 201  and name HB2 ))
  (  segid "BrD " and resid 88   and name HD% )
    2 700      1 800      1.800 peak     46 weight  0.11000E+01 volume  0 13938E+03 ppm1      3 429 ppm2      7.637
OR {   46}
  (( segid "AcH " and resid 201  and name HB1 ))
  (  segid "BrD " and resid 88   and name HD% )
ASSI {   56}
  (( segid "AcH " and resid 201  and name HA2 ))
  (  segid "BrD " and resid 95   and name HE% )
    2.600      1 700      1 700 peak     56 weight  0 11000E+01 volume  0.16075E+03 ppm1      4 015 ppm2      7 585
OR {   56}
  (( segid "AcH " and resid 201  and name HA1 ))
  (  segid "BrD " and resid 95   and name HE% )
ASSI {   66}
  (( segid "AcH " and resid 201  and name HB1 ))
  (  segid "BrD " and resid 95   and name HE% )
    2 600      1 700      1.700 peak     66 weight  0 11000E+01 volume  0 16293E+03 ppm1      3 429 ppm2      7 585
ASSI {   76}
  (  segid "AcH " and resid 200  and name HA% )
  (  segid "BrD " and resid 95   and name HE% )
    2 700      1 800      1 800 peak     76 weight  0 11000E+01 volume  0.14049E+03 ppm1      2 542 ppm2      7.585
ASSI {   86}
  (( segid "AcH " and resid 201  and name HA1 ))
  (  segid "BrD " and resid 88   and name HE% )
    2 600      1 700      1 700 peak     86 weight  0.11000E+01 volume  0 16796E+03 ppm1      4 019 ppm2      7.358
OR {   86}
  (( segid "AcH " and resid 201  and name HA2 ))
  (  segid "BrD " and resid 88   and name HE% )
ASSI {   96}
  (( segid "AcH " and resid 201  and name HB2 ))
  (  segid "BrD " and resid 88   and name HE% )
    2 600      1 700      1 700 peak     96 weight  0.11000E+01 volume  0 16763E+03 ppm1      3.430 ppm2      7 358
OR {   96}
  (( segid "AcH " and resid 201  and name HB1 ))
  (  segid "BrD " and resid 88   and name HE% )
ASSI {    7}
  (  segid "AcH " and resid 200  and name HA% )
  (( segid "AcH " and resid 201  and name HN  ))
    2.700      1 800      1 800 peak      7 weight  0 11000E+01 volume  0 12000E+03 ppm1      3 430 ppm2      7.358
ASSI {   17}
  (  segid "AcH " and resid 200  and name HA% )
  (( segid "AcH " and resid 201  and name HA1 ))
    2.700      1 800      1.800 peak     17 weight  0.11000E+01 volume  0 12000E+03 ppm1      3.430 ppm2      7 358
ASSI {   27}
  (( segid "AcH " and resid 201  and name HB2 ))
  (( segid "AcH " and resid 201  and name HD1 ))
    2.700      1.800      1 800 peak     27 weight  0 11000E+01 volume  0.12000E+03 ppm1      3 430 ppm2      7 358
OR {   27}
  (( segid "AcH " and resid 201  and name HB1 ))
  (( segid "AcH " and resid 201  and name HD1 ))
ASSI {   37}
  (( segid "AcH " and resid 201  and name HB1 ))
  (( segid "AcH " and resid 201  and name HN  ))
    2 700      1 800      1 800 peak     37 weight  0 11000E+01 volume  0 12000E+03 ppm1      3 430 ppm2      7 358
OR {   37}
  (( segid "AcH " and resid 201  and name HB2 ))
  (( segid "AcH " and resid 201  and name HN  ))
ASSI {   47}
  (( segid "AcH " and resid 201  and name HA2 ))
  (( segid "AcH " and resid 201  and name HN  ))
    2 700      1 800      1 800 peak     47 weight  0.11000E+01 volume  0 12000E+03 ppm1      3 430 ppm2      7 358
OR {   47}
  (( segid "AcH " and resid 201  and name HA1 ))
  (( segid "AcH " and resid 201  and name HN  ))
```

Table 3

Ambiguous NOE-derived Inter-proton Distance Restraints

```
ASSI {  311}
  (( segid "BrD " and resid 32   and name HN  ))
  (( segid "BrD " and resid 35   and name HG1 ))
    4 200      4 200      1 300 peak   311 weight  0.10000E+01 volume  0 35526E+02 ppm1       7 738 ppm2       3 430
OR {  311}
  (( segid "BrD " and resid 32   and name HN  ))
  (( segid "BrD " and resid 28   and name HB2 ))
ASSI {  391}
  (( segid "BrD " and resid 106  and name HN  ))
  (  segid "BrD " and resid 105  and name HD% )
    3 100      2 400      2.400 peak   391 weight  0 10000E+01 volume  0 20417E+03 ppm1       9 740 ppm2       7 778
OR {  391}
  (( segid "BrD " and resid 106  and name HN  ))
  (( segid "BrD " and resid 104  and name HN  ))
OR {  391}
  (( segid "BrD " and resid 106  and name HN  ))
  (  segid "BrD " and resid 107  and name HD% )
ASSI {  731}
  (( segid "BrD " and resid 100  and name HN  ))
  (( segid "BrD " and resid 97   and name HA  ))
    3 300      2.700      2 200 peak   731 weight  0 10000E+01 volume  0 15089E+03 ppm1       8 669 ppm2       4 801
OR {  731}
  (( segid "BrD " and resid 100  and name HN  ))
  (( segid "BrD " and resid 98   and name HA  ))
ASSI {  781}
  (( segid "BrD " and resid 97   and name HN  ))
  (( segid "BrD " and resid 98   and name HB2 ))
    4 000      4 000      1 500 peak   781 weight  0 10000E+01 volume  0 45845E+02 ppm1       8 673 ppm2       3 671
OR {  781}
  (( segid "BrD " and resid 97   and name HN  ))
  (( segid "BrD " and resid 85   and name HB2 ))
ASSI {  831}
  (( segid "BrD " and resid 96   and name HN  ))
  (( segid "BrD " and resid 97   and name HB1 ))
    3 200      2 600      2.300 peak   831 weight  0.10000E+01 volume  0 17645E+03 ppm1       7 977 ppm2       2 728
OR {  831}
  (( segid "BrD " and resid 78   and name HN  ))
  (( segid "BrD " and resid 79   and name HB2 ))
OR {  831}
  (( segid "BrD " and resid 77   and name HN  ))
  (( segid "BrD " and resid 79   and name HB2 ))
OR {  831}
  (( segid "BrD " and resid 96   and name HN  ))
  (( segid "BrD " and resid 92   and name HB1 ))
OR {  831}
  (( segid "BrD " and resid 78   and name HN  ))
  (( segid "BrD " and resid 79   and name HB1 ))
ASSI { 1051}
  (( segid "BrD " and resid 76   and name HN  ))
  (( segid "BrD " and resid 73   and name HB2 ))
    5 000      5 000      0.500 peak  1051 weight  0 10000E+01 volume  0 12021E+02 ppm1       8 612 ppm2       2 497
OR { 1051}
  (( segid "BrD " and resid 76   and name HN  ))
  (( segid "BrD " and resid 80   and name HB2 ))
ASSI { 1101}
  (( segid "BrD " and resid 75   and name HN  ))
  (( segid "BrD " and resid 18   and name HG  ))
    5 500      5 500      0.000 peak  1101 weight  0 10000E+01 volume  0 63178E+01 ppm1       9 107 ppm2       2 294
OR { 1101}
  (( segid "BrD " and resid 75   and name HN  ))
  (( segid "BrD " and resid 72   and name HD1 ))
OR { 1101}
  (( segid "BrD " and resid 98   and name HN  ))
  (  segid "BrD " and resid 31   and name HB% )
ASSI { 1551}
  (( segid "BrD " and resid 21   and name HN  ))
  (( segid "BrD " and resid 24   and name HE22))
    3 400      2.900      2 100 peak  1551 weight  0 10000E+01 volume  0 12608E+03 ppm1       8 544 ppm2       7.515
OR { 1551}
  (( segid "BrD " and resid 21   and name HN  ))
  (  segid "BrD " and resid 106  and name HD% )
OR { 1551}
  (( segid "BrD " and resid 109  and name HN  ))
  (  segid "BrD " and resid 106  and name HD% )
OR { 1551}
  (( segid "BrD " and resid 64   and name HN  ))
  (  segid "BrD " and resid 15   and name HE% )
ASSI { 1781}
  (( segid "BrD " and resid 26   and name HN  ))
  (( segid "BrD " and resid 22   and name HB1 ))
    3.400      2.900      2 100 peak  1781 weight  0 10000E+01 volume  0.12549E+03 ppm1       9 196 ppm2       2 672
OR { 1781}
  (( segid "BrD " and resid 26   and name HN  ))
  (( segid "BrD " and resid 56   and name HB1 ))
ASSI { 2721}
  (( segid "BrD " and resid 104  and name HN  ))
  (( segid "BrD " and resid 105  and name HB2 ))
    3 300      2 700      2 200 peak  2721 weight  0 10000E+01 volume  0 14753E+03 ppm1       7 763 ppm2       3 671
OR { 2721}
  (( segid "BrD " and resid 104  and name HN  ))
  (( segid "BrD " and resid 107  and name HB1 ))
OR { 2721}
  (( segid "BrD " and resid 104  and name HN  ))
  (( segid "BrD " and resid 106  and name HB2 ))
ASSI { 3261}
  (( segid "BrD " and resid 16   and name HN  ))
  (( segid "BrD " and resid 13   and name HG2 ))
    4 100      4 100      1 400 peak  3261 weight  0.10000E+01 volume  0 41938E+02 ppm1       8 794 ppm2       2.954
OR { 3261}
  (( segid "BrD " and resid 16   and name HN  ))
  (( segid "BrD " and resid 11   and name HB1 ))
ASSI { 3361}
  (( segid "BrD " and resid 13   and name HN  ))
  (( segid "BrD " and resid 13   and name HG1 ))
    4 100      4 100      1 400 peak  3361 weight  0.10000E+01 volume  0.40202E+02 ppm1       8.809 ppm2       3 103
OR { 3361}
  (( segid "BrD " and resid 14   and name HN  ))
  (( segid "BrD " and resid 13   and name HG1 ))
ASSI { 3371}
  (( segid "BrD " and resid 13   and name HN  ))
  (( segid "BrD " and resid 13   and name HG2 ))
    3 300      2 700      2 200 peak  3371 weight  0 10000E+01 volume  0 14859E+03 ppm1       8 802 ppm2       2 987
OR { 3371}
  (( segid "BrD " and resid 14   and name HN  ))
  (( segid "BrD " and resid 13   and name HG2 ))
ASSI { 3401}
  (( segid "BrD " and resid 13   and name HN  ))
  (( segid "BrD " and resid 11   and name HD1 ))
    3 800      3 600      1 700 peak  3401 weight  0 10000E+01 volume  0.67241E+02 ppm1       8 810 ppm2       4.488
OR { 3401}
  (( segid "BrD " and resid 14   and name HN  ))
  (( segid "BrD " and resid 11   and name HD1 ))
OR { 3401}
  (( segid "BrD " and resid 14   and name HN  ))
  (( segid "BrD " and resid 16   and name HA  ))
ASSI { 3671}
  (( segid "BrD " and resid 102  and name HN  ))
  (( segid "BrD " and resid 30   and name HB1 ))
    3 800      3 600      1.700 peak  3671 weight  0 10000E+01 volume  0 58619E+02 ppm1       9 156 ppm2       4 934
OR { 3671}
  (( segid "BrD " and resid 102  and name HN  ))
  (( segid "BrD " and resid 100  and name HA  ))
ASSI { 3841}
  (( segid "BrD " and resid 103  and name HN  ))
  (( segid "BrD " and resid 100  and name HA  ))
    3 000      2 200      2 200 peak  3841 weight  0 10000E+01 volume  0.24821E+03 ppm1       8 661 ppm2       4 900
OR { 3841}
  (( segid "BrD " and resid 40   and name HN  ))
  (( segid "BrD " and resid 41   and name HB  ))
ASSI { 3911}
  (( segid "BrD " and resid 59   and name HN  ))
  (( segid "BrD " and resid 57   and name HB1 ))
    3 500      3 100      2 000 peak  3911 weight  0 10000E+01 volume  0 98690E+02 ppm1       8 496 ppm2       2 969
OR { 3911}
  (( segid "BrD " and resid 59   and name HN  ))
  (( segid "BrD " and resid 61   and name HG1 ))
OR { 3911}
  (( segid "BrD " and resid 31   and name HN  ))
  (( segid "BrD " and resid 29   and name HG1 ))
OR { 3911}
  (( segid "BrD " and resid 59   and name HN  ))
  (( segid "BrD " and resid 55   and name HB1 ))
ASSI { 4131}
  (( segid "BrD " and resid 25   and name HN  ))
  (( segid "BrD " and resid 21   and name HB  ))
    3 800      3 600      1.700 peak  4131 weight  0 10000E+01 volume  0 59139E+02 ppm1       9 133 ppm2       2 465
OR { 4131}
  (( segid "BrD " and resid 25   and name HN  ))
  (( segid "BrD " and resid 26   and name HB1 ))
ASSI { 6751}
  (( segid "BrD " and resid 111  and name HN  ))
  (( segid "BrD " and resid 111  and name HD1 ))
    3 200      2 600      2.300 peak  6751 weight  0.10000E+01 volume  0 16212E+03 ppm1       8 168 ppm2       2.204
OR { 6751}
  (( segid "BrD " and resid 111  and name HN  ))
  (( segid "BrD " and resid 109  and name HB2 ))
ASSI { 6861}
  (( segid "BrD " and resid 21   and name HN  ))
  (( segid "BrD " and resid 24   and name HG2 ))
    3 400      2 900      2 100 peak  6861 weight  0 10000E+01 volume  0.12194E+03 ppm1       8 574 ppm2       3 072
OR { 6861}
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   (( segid "BrD " and resid 21   and name HN  ))
   (( segid "BrD " and resid 24   and name HB2 ))
OR { 6861}
   (( segid "BrD " and resid 21   and name HN  ))
   (( segid "BrD " and resid 23   and name HG2 ))
OR { 6861}
   (( segid "BrD " and resid 21   and name HN  ))
   (( segid "BrD " and resid 24   and name HB1 ))
ASSI { 6871}
   (( segid "BrD " and resid 21   and name HN  ))
   (( segid "BrD " and resid 22   and name HB1 ))
     3 300      2 700      2 200 peak  6871 weight  0 10000E+01 volume  0 15992E+03 ppm1      8 573 ppm2      2 702
OR { 6871}
   (( segid "BrD " and resid 64   and name HN  ))
   (( segid "BrD " and resid 61   and name HB2 ))
OR { 6871}
   (( segid "BrD " and resid 109  and name HN  ))
   (( segid "BrD " and resid 112  and name HB1 ))
OR { 6871}
   (( segid "BrD " and resid 64   and name HN  ))
   (( segid "BrD " and resid 22   and name HB1 ))
ASSI { 6911}
   (( segid "BrD " and resid 86   and name HN  ))
   (( segid "BrD " and resid 86   and name HE1 ))
     3.700      3 400      1 800 peak  6911 weight  0 10000E+01 volume  0 78171E+02 ppm1      8 423 ppm2      3 044
OR { 6911}
   (( segid "BrD " and resid 86   and name HN  ))
   (( segid "BrD " and resid 87   and name HG1 ))
ASSI { 7031}
   (( segid "BrD " and resid 52   and name HN  ))
   (( segid "BrD " and resid 80   and name HN  ))
     4 200      4 200      1 300 peak  7031 weight  0 10000E+01 volume  0 35356E+02 ppm1      9 003 ppm2      7 979
OR { 7031}
   (( segid "BrD " and resid 52   and name HN  ))
   (( segid "BrD " and resid 77   and name HN  ))
OR { 7031}
   (( segid "BrD " and resid 52   and name HN  ))
   (  segid "BrD " and resid 47   and name HD% )
ASSI { 7121}
   (( segid "BrD " and resid 89   and name HD21))
   (( segid "BrD " and resid 85   and name HA  ))
     3 700      3 400      1 800 peak  7121 weight  0.10000E+01 volume  0 76700E+02 ppm1      8 923 ppm2      5 021
OR { 7121}
   (( segid "BrD " and resid 89   and name HD21))
   (( segid "BrD " and resid 93   and name HB1 ))
ASSI { 7131}
   (( segid "BrD " and resid 89   and name HD22))
   (( segid "BrD " and resid 85   and name HA  ))
     3.600      3 200      1 900 peak  7131 weight  0 10000E+01 volume  0 84076E+02 ppm1      8 416 ppm2      5 021
OR { 7131}
   (( segid "BrD " and resid 89   and name HD22))
   (( segid "BrD " and resid 93   and name HB1 ))
ASSI { 7251}
   (( segid "BrD " and resid 26   and name HN  ))
   (  segid "BrD " and resid 22   and name HD2% )
     3 000      2 200      2 200 peak  7251 weight  0 10000E+01 volume  0 24489E+03 ppm1      9 196 ppm2      1 549
OR { 7251}
   (( segid "BrD " and resid 26   and name HN  ))
   (  segid "BrD " and resid 56   and name HD1% )
ASSI { 8181}
   (( segid "BrD " and resid 57   and name HN  ))
   (  segid "BrD " and resid 25   and name HG2% )
     4.100      4 100      1 400 peak  8181 weight  0 10000E+01 volume  0 42960E+02 ppm1      9 359 ppm2      1 667
OR { 8181}
   (( segid "BrD " and resid 57   and name HN  ))
   (  segid "BrD " and resid 58   and name HG2% )
OR { 8181}
   (( segid "BrD " and resid 57   and name HN  ))
   (  segid "BrD " and resid 22   and name HD1% )
ASSI { 8211}
   (( segid "BrD " and resid 114  and name HN  ))
   (( segid "BrD " and resid 111  and name HB2 ))
     4 000      4 000      1 500 peak  8211 weight  0.10000E+01 volume  0 47918E+02 ppm1      8.377 ppm2      2 377
OR { 8211}
   (( segid "BrD " and resid 114  and name HN  ))
   (( segid "BrD " and resid 110  and name HB  ))
ASSI { 8261}
   (( segid "BrD " and resid 28   and name HN  ))
   (( segid "BrD " and resid 25   and name HB  ))
     4 200      4 200      1 300 peak  8261 weight  0.10000E+01 volume  0 36987E+02 ppm1      8 166 ppm2      3 014
OR { 8261}
   (( segid "BrD " and resid 28   and name HN  ))
   (( segid "BrD " and resid 29   and name HG1 ))
ASSI { 8291}
   (( segid "BrD " and resid 28   and name HN  ))
   (  segid "BrD " and resid 25   and name HG2% )
     4 400      4 400      1.100 peak  8291 weight  0.10000E+01 volume  0 24897E+02 ppm1      8 164 ppm2      1 639
OR { 8291}
   (( segid "BrD " and resid 28   and name HN  ))
   (( segid "BrD " and resid 26   and name HG1 ))
ASSI { 8381}
   (( segid "BrD " and resid 61   and name HN  ))
   (  segid "BrD " and resid 58   and name HG2% )
     3.400      2 900      2 100 peak  8381 weight  0 10000E+01 volume  0 13119E+03 ppm1      8 743 ppm2      1 674
OR { 8381}
   (( segid "BrD " and resid 61   and name HN  ))
   (  segid "BrD " and resid 22   and name HD1% )
OR { 8381}
   (( segid "BrD " and resid 38   and name HN  ))
   (  segid "BrD " and resid 43   and name HB% )
ASSI { 8391}
   (( segid "BrD " and resid 38   and name HN  ))
   (( segid "BrD " and resid 39   and name HG1 ))
     4 000      4.000      1 500 peak  8391 weight  0 10000E+01 volume  0.45211E+02 ppm1      8 743 ppm2      2.008
OR { 8391}
   (( segid "BrD " and resid 61   and name HN  ))
   (( segid "BrD " and resid 57   and name HG2 ))
ASSI { 8511}
   (( segid "BrD " and resid 50   and name HN  ))
   (( segid "BrD " and resid 53   and name HG1 ))
     3 700      3 400      1.800 peak  8511 weight  0.10000E+01 volume  0 70210E+02 ppm1      8 564 ppm2      2 814
OR { 8511}
   (( segid "BrD " and resid 50   and name HN  ))
   (( segid "BrD " and resid 53   and name HB1 ))
OR { 8511}
   (( segid "BrD " and resid 50   and name HN  ))
   (( segid "BrD " and resid 87   and name HB1 ))
OR { 8511}
   (( segid "BrD " and resid 46   and name HN  ))
   (( segid "BrD " and resid 53   and name HG1 ))
OR { 8511}
   (( segid "BrD " and resid 46   and name HN  ))
   (( segid "BrD " and resid 53   and name HB1 ))
ASSI { 8751}
   (( segid "BrD " and resid 58   and name HN  ))
   (( segid "BrD " and resid 37   and name HG1 ))
     3 400      2 900      2 100 peak  8751 weight  0 10000E+01 volume  0 12911E+03 ppm1     10 051 ppm2      2 747
OR { 8751}
   (( segid "BrD " and resid 58   and name HN  ))
   (  segid "BrD " and resid 35   and name HE% )
ASSI { 8861}
   (( segid "BrD " and resid 9    and name HN  ))
   (( segid "BrD " and resid 8    and name HG1 ))
     3 600      3 200      1 900 peak  8861 weight  0 10000E+01 volume  0 86153E+02 ppm1      9 052 ppm2      2.631
OR { 8861}
   (( segid "BrD " and resid 9    and name HN  ))
   (( segid "BrD " and resid 7    and name HB1 ))
ASSI { 8891}
   (( segid "BrD " and resid 103  and name HN  ))
   (( segid "BrD " and resid 100  and name HA  ))
     4 000      4.000      1 500 peak  8891 weight  0 10000E+01 volume  0 44524E+02 ppm1      8 668 ppm2      4 917
OR { 8891}
   (( segid "BrD " and resid 112  and name HN  ))
   (( segid "BrD " and resid 113  and name HA  ))
ASSI { 8901}
   (( segid "BrD " and resid 112  and name HN  ))
   (( segid "BrD " and resid 108  and name HA  ))
     3 400      2 900      2.100 peak  8901 weight  0 10000E+01 volume  0 11279E+03 ppm1      8.668 ppm2      4 805
OR { 8901}
   (( segid "BrD " and resid 103  and name HN  ))
   (( segid "BrD " and resid 82   and name HA  ))
OR { 8901}
   (( segid "BrD " and resid 103  and name HN  ))
   (( segid "BrD " and resid 98   and name HA  ))
ASSI { 8911}
   (( segid "BrD " and resid 103  and name HN  ))
   (( segid "BrD " and resid 99   and name HA  ))
     3 500      3 100      2 000 peak  8911 weight  0.10000E+01 volume  0 10762E+03 ppm1      8 668 ppm2      4 426
OR { 8911}
   (( segid "BrD " and resid 112  and name HN  ))
   (( segid "BrD " and resid 110  and name HA  ))
ASSI { 8941}
   (( segid "BrD " and resid 103  and name HN  ))
   (  segid "BrD " and resid 99   and name HB% )
     2 900      2.100      2 100 peak  8941 weight  0 10000E+01 volume  0 29817E+03 ppm1      8 667 ppm2      2 178
OR { 8941}
   (( segid "BrD " and resid 103  and name HN  ))
   (( segid "BrD " and resid 102  and name HG  ))
OR { 8941}
   (( segid "BrD " and resid 112  and name HN  ))
   (( segid "BrD " and resid 109  and name HB2 ))
ASSI { 9011}
   (( segid "BrD " and resid 105  and name HN  ))
   (( segid "BrD " and resid 104  and name HD1 ))
     3 100      2.400      2 400 peak  9011 weight  0 10000E+01 volume  0.22428E+03 ppm1      8 487 ppm2      2.294
OR { 9011}
   (( segid "BrD " and resid 105  and name HN  ))
   (( segid "BrD " and resid 103  and name HB1 ))
ASSI { 9031}
   (( segid "BrD " and resid 105  and name HN  ))
   (( segid "BrD " and resid 102  and name HB2 ))
     3 800      3.600      1 700 peak  9031 weight  0 10000E+01 volume  0.62331E+02 ppm1      8 487 ppm2      1 805
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 OR { 9031}
   (( segid "BrD " and resid 105  and name HN  ))
   (  segid "BrD " and resid 25   and name HG1%)
 ASSI { 9091}
   (( segid "BrD " and resid 109  and name HN  ))
   (( segid "BrD " and resid 106  and name HB2 ))
      3 800     3.600     1 700 peak  9091 weight  0 10000E+01 volume  0 66318E+02 ppm1      8 574 ppm2      3 678
 OR { 9091}
   (( segid "BrD " and resid 109  and name HN  ))
   (( segid "BrD " and resid 107  and name HB1 ))
 OR { 9091}
   (( segid "BrD " and resid 109  and name HN  ))
   (( segid "BrD " and resid 105  and name HB2 ))
 OR { 9091}
   (( segid "BrD " and resid 64   and name HN  ))
   (( segid "BrD " and resid 68   and name HB1 ))
 ASSI { 9101}
   (( segid "BrD " and resid 64   and name HN  ))
   (( segid "BrD " and resid 63   and name HB3 ))
      2 900     2 100     2 100 peak  9101 weight  0 10000E+01 volume  0 30416E+03 ppm1      8 573 ppm2      2 498
 OR { 9101}
   (( segid "BrD " and resid 21   and name HN  ))
   (( segid "BrD " and resid 21   and name HB  ))
 ASSI { 9111}
   (( segid "BrD " and resid 21   and name HN  ))
   (  segid "BrD " and resid 17   and name HG2%)
      3 500     3 100     2 000 peak  9111 weight  0 10000E+01 volume  0 10029E+03 ppm1      8 574 ppm2      1 725
 OR { 9111}
   (( segid "BrD " and resid 109  and name HN  ))
   (  segid "BrD " and resid 17   and name HG2%)
 ASSI { 9161}
   (( segid "BrD " and resid 106  and name HN  ))
   (( segid "BrD " and resid 104  and name HB1 ))
      3 900     3 800     1 600 peak  9161 weight  0 10000E+01 volume  0 56197E+02 ppm1      9 740 ppm2      2.560
 OR { 9161}
   (( segid "BrD " and resid 106  and name HN  ))
   (( segid "BrD " and resid 103  and name HG2 ))
 ASSI { 9171}
   (( segid "BrD " and resid 106  and name HN  ))
   (( segid "BrD " and resid 109  and name HB1 ))
      4 000     4 000     1 500 peak  9171 weight  0 10000E+01 volume  0 47295E+02 ppm1      9 739 ppm2      2 318
 OR { 9171}
   (( segid "BrD " and resid 106  and name HN  ))
   (( segid "BrD " and resid 103  and name HB1 ))
 OR { 9171}
   (( segid "BrD " and resid 106  and name HN  ))
   (( segid "BrD " and resid 104  and name HD1 ))
 OR { 9171}
   (( segid "BrD " and resid 106  and name HN  ))
   (( segid "BrD " and resid 21   and name HG11))
 ASSI { 9181}
   (( segid "BrD " and resid 106  and name HN  ))
   (( segid "BrD " and resid 102  and name HG  ))
      4 100     4.100     1 400 peak  9181 weight  0 10000E+01 volume  0 40041E+02 ppm1      9 742 ppm2      2 150
 OR { 9181}
   (( segid "BrD " and resid 106  and name HN  ))
   (( segid "BrD " and resid 109  and name HB2 ))
 ASSI { 9191}
   (( segid "BrD " and resid 106  and name HN  ))
   (( segid "BrD " and resid 102  and name HB1 ))
      4 200     4 200     1 300 peak  9191 weight  0 10000E+01 volume  0 35794E+02 ppm1      9 740 ppm2      2.002
 OR { 9191}
   (( segid "BrD " and resid 106  and name HN  ))
   (( segid "BrD " and resid 109  and name HD1 ))
 ASSI { 9201}
   (( segid "BrD " and resid 106  and name HN  ))
   (( segid "BrD " and resid 102  and name HB2 ))
      3 900     3.800     1 600 peak  9201 weight  0 10000E+01 volume  0.56492E+02 ppm1      9 739 ppm2      1.786
 OR { 9201}
   (( segid "BrD " and resid 106  and name HN  ))
   (  segid "BrD " and resid 25   and name HG1%)
 ASSI { 9241}
   (( segid "BrD " and resid 84   and name HN  ))
   (( segid "BrD " and resid 80   and name HD2 ))
      3 700     3.400     1 800 peak  9241 weight  0 10000E+01 volume  0 69670E+02 ppm1      9.464 ppm2      3 908
 OR { 9241}
   (( segid "BrD " and resid 84   and name HN  ))
   (( segid "BrD " and resid 85   and name HB1 ))
 ASSI { 9251}
   (( segid "BrD " and resid 63   and name HN  ))
   (( segid "BrD " and resid 62   and name HG1 ))
      3 700     3 400     1 800 peak  9251 weight  0.10000E+01 volume  0 78060E+02 ppm1      9 463 ppm2      2 352
 OR { 9251}
   (( segid "BrD " and resid 84   and name HN  ))
   (( segid "BrD " and resid 80   and name HG1 ))
 OR { 9251}
   (( segid "BrD " and resid 84   and name HN  ))
   (( segid "BrD " and resid 86   and name HB1 ))
 ASSI { 9281}
   (( segid "BrD " and resid 84   and name HN  ))
   (( segid "BrD " and resid 80   and name HN  ))
      3 300     2 700     2 200 peak  9281 weight  0 10000E+01 volume  0 13642E+03 ppm1      9 462 ppm2      8.001
 OR { 9281}
   (( segid "BrD " and resid 84   and name HN  ))
   (( segid "BrD " and resid 107  and name HZ  ))
 OR { 9281}
   (( segid "BrD " and resid 63   and name HN  ))
   (( segid "BrD " and resid 70   and name HN  ))
 ASSI { 9311}
   (( segid "BrD " and resid 22   and name HN  ))
   (( segid "BrD " and resid 22   and name HA  ))
      4 200     4 200     1.300 peak  9311 weight  0 10000E+01 volume  0 35671E+02 ppm1      9 472 ppm2      4 678
 OR { 9311}
   (( segid "BrD " and resid 84   and name HN  ))
   (( segid "BrD " and resid 80   and name HA  ))
 ASSI { 9341}
   (( segid "BrD " and resid 63   and name HN  ))
   (  segid "BrD " and resid 74   and name HB% )
      2 900     2 100     2 100 peak  9341 weight  0 10000E+01 volume  0 30219E+03 ppm1      9 456 ppm2      7 530
 OR { 9341}
   (( segid "BrD " and resid 22   and name HN  ))
   (  segid "BrD " and resid 106  and name HD% )
 ASSI { 9371}
   (( segid "BrD " and resid 22   and name HN  ))
   (( segid "BrD " and resid 24   and name HG2 ))
      3 400     2 900     2 100 peak  9371 weight  0 10000E+01 volume  0 12105E+03 ppm1      9 456 ppm2      3 066
 OR { 9371}
   (( segid "BrD " and resid 22   and name HN  ))
   (( segid "BrD " and resid 23   and name HG2 ))
 OR { 9371}
   (( segid "BrD " and resid 63   and name HN  ))
   (( segid "BrD " and resid 59   and name HG2 ))
 ASSI { 9441}
   (( segid "BrD " and resid 109  and name HN  ))
   (( segid "BrD " and resid 109  and name HB2 ))
      3 900     3 800     1 600 peak  9441 weight  0 10000E+01 volume  0 55505E+02 ppm1      8 557 ppm2      2 173
 OR { 9441}
   (( segid "BrD " and resid 64   and name HN  ))
   (( segid "BrD " and resid 64   and name HG1 ))
 ASSI { 9451}
   (( segid "BrD " and resid 21   and name HN  ))
   (( segid "BrD " and resid 24   and name HG2 ))
      3 900     3 800     1 600 peak  9451 weight  0 10000E+01 volume  0 53501E+02 ppm1      8 556 ppm2      3 108
 OR { 9451}
   (( segid "BrD " and resid 21   and name HN  ))
   (( segid "BrD " and resid 24   and name HB2 ))
 OR { 9451}
   (( segid "BrD " and resid 21   and name HN  ))
   (( segid "BrD " and resid 23   and name HG1 ))
 OR { 9451}
   (( segid "BrD " and resid 21   and name HN  ))
   (( segid "BrD " and resid 24   and name HB1 ))
 ASSI { 9461}
   (( segid "BrD " and resid 64   and name HN  ))
   (( segid "BrD " and resid 61   and name HB1 ))
      3 700     3 400     1 800 peak  9461 weight  0 10000E+01 volume  0.72347E+02 ppm1      8 544 ppm2      2 851
 OR { 9461}
   (( segid "BrD " and resid 21   and name HN  ))
   (( segid "BrD " and resid 23   and name HB2 ))
 ASSI { 9491}
   (( segid "BrD " and resid 21   and name HN  ))
   (( segid "BrD " and resid 19   and name HB2 ))
      3 300     2 700     2.200 peak  9491 weight  0 10000E+01 volume  0.14127E+03 ppm1      8.556 ppm2      1 929
 OR { 9491}
   (( segid "BrD " and resid 109  and name HN  ))
   (( segid "BrD " and resid 111  and name HG2 ))
 OR { 9491}
   (( segid "BrD " and resid 109  and name HN  ))
   (  segid "BrD " and resid 113  and name HB% )
 OR { 9491}
   (( segid "BrD " and resid 64   and name HN  ))
   (( segid "BrD " and resid 19   and name HB2 ))
 ASSI { 9501}
   (( segid "BrD " and resid 21   and name HN  ))
   (  segid "BrD " and resid 17   and name HG2%)
      3 300     2 700     2 200 peak  9501 weight  0 10000E+01 volume  0 14396E+03 ppm1      8 556 ppm2      1 762
 OR { 9501}
   (( segid "BrD " and resid 109  and name HN  ))
   (  segid "BrD " and resid 17   and name HG2%)
 OR { 9501}
   (( segid "BrD " and resid 21   and name HN  ))
   (  segid "BrD " and resid 25   and name HG1%)
 ASSI { 9531}
   (( segid "BrD " and resid 17   and name HN  ))
   (( segid "BrD " and resid 13   and name HA  ))
      3 600     3 200     1 900 peak  9531 weight  0 10000E+01 volume  0.86367E+02 ppm1      8.695 ppm2      4 805
 OR { 9531}
   (( segid "BrD " and resid 112  and name HN  ))
   (( segid "BrD " and resid 108  and name HA  ))
 OR { 9531}
   (( segid "BrD " and resid 103  and name HN  ))
   (( segid "BrD " and resid 82   and name HA  ))
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ASSI { 9561}
  (( segid "BrD " and resid 103  and name HN  ))
  (( segid "BrD " and resid 106  and name HB2 ))
    3 300     2 700     2 200 peak  9561 weight  0 10000E+01 volume  0 15504E+03 ppm1      8 696 ppm2      3 661
OR { 9561}
  (( segid "BrD " and resid 103  and name HN  ))
  (( segid "BrD " and resid 82   and name HB1 ))
OR { 9561}
  (( segid "BrD " and resid 103  and name HN  ))
  (( segid "BrD " and resid 105  and name HB2 ))
OR { 9561}
  (( segid "BrD " and resid 103  and name HN  ))
  (( segid "BrD " and resid 107  and name HB1 ))
ASSI { 9631}
  (( segid "BrD " and resid 99   and name HN  ))
  (( segid "BrD " and resid 100  and name HA  ))
    3 900     3 800     1 600 peak  9631 weight  0 10000E+01 volume  0 54041E+02 ppm1      8 936 ppm2      4 947
OR { 9631}
  (( segid "BrD " and resid 99   and name HN  ))
  (( segid "BrD " and resid 30   and name HB1 ))
ASSI { 9641}
  (( segid "BrD " and resid 99   and name HN  ))
  (( segid "BrD " and resid 101  and name HG11))
    3 900     3 800     1 600 peak  9641 weight  0 10000E+01 volume  0 56248E+02 ppm1      8 935 ppm2      2 460
OR { 9641}
  (( segid "BrD " and resid 99   and name HN  ))
  (( segid "BrD " and resid 97   and name HG1 ))
ASSI { 9651}
  (( segid "BrD " and resid 99   and name HN  ))
  (( segid "BrD " and resid 103  and name HB2 ))
    5 500     5 500     0 000 peak  9651 weight  0 10000E+01 volume  0 57216E-02 ppm1      8 936 ppm2      1 920
OR { 9651}
  (( segid "BrD " and resid 99   and name HN  ))
  (( segid "BrD " and resid 86   and name HG1 ))
ASSI { 9721}
  (( segid "BrD " and resid 64   and name HN  ))
  (( segid "BrD " and resid 64   and name HE1 ))
    4 000     4 000     1 500 peak  9721 weight  0 10000E+01 volume  0.46621E+02 ppm1      8 586 ppm2      3 626
OR { 9721}
  (( segid "BrD " and resid 64   and name HN  ))
  (( segid "BrD " and resid 65   and name HB1 ))
ASSI { 9731}
  (( segid "BrD " and resid 21   and name HN  ))
  (( segid "BrD " and resid 109  and name HE1 ))
    3 800     3 600     1 700 peak  9731 weight  0 10000E+01 volume  0.59335E+02 ppm1      8.584 ppm2      3 146
OR { 9731}
  (( segid "BrD " and resid 21   and name HN  ))
  (( segid "BrD " and resid 23   and name HG1 ))
ASSI { 9801}
  (( segid "BrD " and resid 103  and name HN  ))
  (( segid "BrD " and resid 106  and name HB2 ))
    4 600     4 600     0 900 peak  9801 weight  0 10000E+01 volume  0 19838E+02 ppm1      8 669 ppm2      3.659
OR { 9801}
  (( segid "BrD " and resid 17   and name HN  ))
  (( segid "BrD " and resid 15   and name HB2 ))
OR { 9801}
  (( segid "BrD " and resid 103  and name HN  ))
  (( segid "BrD " and resid 82   and name HB1 ))
OR { 9801}
  (( segid "BrD " and resid 103  and name HN  ))
  (( segid "BrD " and resid 105  and name HB2 ))
ASSI { 9821}
  (( segid "BrD " and resid 17   and name HN  ))
  (( segid "BrD " and resid 13   and name HG2 ))
    3 700     3 400     1.800 peak  9821 weight  0 10000E+01 volume  0 70791E+02 ppm1      8 668 ppm2      2 943
OR { 9821}
  (( segid "BrD " and resid 17   and name HN  ))
  (( segid "BrD " and resid 11   and name HB1 ))
ASSI { 9831}
  (( segid "BrD " and resid 17   and name HN  ))
  (( segid "BrD " and resid 18   and name HG  ))
    3 000     2 200     2 200 peak  9831 weight  0.10000E+01 volume  0 24267E+03 ppm1      8 669 ppm2      2 284
OR { 9831}
  (( segid "BrD " and resid 40   and name HN  ))
  (( segid "BrD " and resid 39   and name HD1 ))
OR { 9831}
  (( segid "BrD " and resid 103  and name HN  ))
  (( segid "BrD " and resid 104  and name HD1 ))
ASSI { 9841}
  (( segid "BrD " and resid 103  and name HN  ))
  (( segid "BrD " and resid 102  and name HB1 ))
    4 500     4.500     1.000 peak  9841 weight  0 10000E+01 volume  0.24419E+02 ppm1      8.669 ppm2      1.973
OR { 9841}
  (( segid "BrD " and resid 17   and name HN  ))
  (  segid "BrD " and resid 113  and name HB% )
ASSI { 9861}
  (( segid "BrD " and resid 17   and name HN  ))
  (( segid "BrD " and resid 14   and name HB2 ))
    3 500     3 100     2 000 peak  9861 weight  0.10000E+01 volume  0 99899E+02 ppm1      8.668 ppm2      2 135
OR { 9861}
  (( segid "BrD " and resid 17   and name HN  ))
  (( segid "BrD " and resid 18   and name HB1 ))
OR { 9861}
  (( segid "BrD " and resid 103  and name HN  ))
  (( segid "BrD " and resid 104  and name HG1 ))
ASSI {10081}
  (( segid "BrD " and resid 24   and name HN  ))
  (( segid "BrD " and resid 21   and name HB  ))
    4.300     4 300     1.200 peak 10081 weight  0 10000E+01 volume  0 28058E+02 ppm1      8 666 ppm2      2 481
OR {10081}
  (( segid "BrD " and resid 24   and name HN  ))
  (( segid "BrD " and resid 26   and name HB1 ))
ASSI {10181}
  (( segid "BrD " and resid 16   and name HN  ))
  (( segid "BrD " and resid 14   and name HB2 ))
    4 100     4 100     1 400 peak 10181 weight  0 10000E+01 volume  0 40626E+02 ppm1      8 785 ppm2      2 129
OR {10181}
  (( segid "BrD " and resid 16   and name HN  ))
  (( segid "BrD " and resid 18   and name HB1 ))
ASSI {10201}
  (( segid "BrD " and resid 16   and name HN  ))
  (( segid "BrD " and resid 19   and name HB2 ))
    3 900     3 800     1 600 peak 10201 weight  0 10000E+01 volume  0 57921E+02 ppm1      8 791 ppm2      1 963
OR {10201}
  (( segid "BrD " and resid 16   and name HN  ))
  (  segid "BrD " and resid 113  and name HB% )
ASSI {10241}
  (( segid "BrD " and resid 75   and name HN  ))
  (( segid "BrD " and resid 78   and name HB1 ))
    3 900     3.800     1 600 peak 10241 weight  0 10000E+01 volume  0 50050E+02 ppm1      9 106 ppm2      1 347
OR {10241}
  (( segid "BrD " and resid 75   and name HN  ))
  (  segid "BrD " and resid 115  and name HD1%)
ASSI {10281}
  (( segid "BrD " and resid 98   and name HN  ))
  (( segid "BrD " and resid 97   and name HG1 ))
    4 000     4 000     1 500 peak 10281 weight  0.10000E+01 volume  0 43323E+02 ppm1      9 106 ppm2      2 456
OR {10281}
  (( segid "BrD " and resid 98   and name HN  ))
  (( segid "BrD " and resid 97   and name HD1 ))
OR {10281}
  (( segid "BrD " and resid 98   and name HN  ))
  (( segid "BrD " and resid 101  and name HG11))
ASSI {10331}
  (( segid "BrD " and resid 96   and name HN  ))
  (( segid "BrD " and resid 97   and name HG1 ))
    3 900     3 800     1.600 peak 10331 weight  0.10000E+01 volume  0 52285E+02 ppm1      7 977 ppm2      2 412
OR {10331}
  (( segid "BrD " and resid 77   and name HN  ))
  (( segid "BrD " and resid 73   and name HG  ))
OR {10331}
  (( segid "BrD " and resid 96   and name HN  ))
  (( segid "BrD " and resid 97   and name HD1 ))
OR {10331}
  (( segid "BrD " and resid 77   and name HN  ))
  (( segid "BrD " and resid 72   and name HB1 ))
ASSI {10381}
  (( segid "BrD " and resid 78   and name HN  ))
  (( segid "BrD " and resid 116  and name HG11))
    3 900     3 800     1 600 peak 10381 weight  0 10000E+01 volume  0 51654E+02 ppm1      7 996 ppm2      1 888
OR {10381}
  (( segid "BrD " and resid 77   and name HN  ))
  (( segid "BrD " and resid 116  and name HG11))
ASSI {10391}
  (( segid "BrD " and resid 78   and name HN  ))
  (  segid "BrD " and resid 22   and name HD2%)
    3 500     3.100     2 000 peak 10391 weight  0.10000E+01 volume  0 99200E+02 ppm1      7 996 ppm2      1 604
OR {10391}
  (( segid "BrD " and resid 55   and name HN  ))
  (  segid "BrD " and resid 22   and name HD2%)
OR {10391}
  (( segid "BrD " and resid 78   and name HN  ))
  (  segid "BrD " and resid 25   and name HG2%)
OR {10391}
  (( segid "BrD " and resid 77   and name HN  ))
  (  segid "BrD " and resid 22   and name HD2%)
OR {10391}
  (( segid "BrD " and resid 55   and name HN  ))
  (  segid "BrD " and resid 25   and name HG2%)
ASSI {10411}
  (( segid "BrD " and resid 77   and name HN  ))
  (( segid "BrD " and resid 80   and name HB2 ))
    2 800     2 000     2 000 peak 10411 weight  0 10000E+01 volume  0 43395E+03 ppm1      7 996 ppm2      2 456
OR {10411}
  (( segid "BrD " and resid 78   and name HN  ))
  (( segid "BrD " and resid 80   and name HB2 ))
ASSI {10431}
  (( segid "BrD " and resid 55   and name HN  ))
  (( segid "BrD " and resid 37   and name HG1 ))
    2 600     1 700     1.700 peak 10431 weight  0 10000E+01 volume  0.60264E+03 ppm1      7 996 ppm2      2 722
OR {10431}
  (( segid "BrD " and resid 78   and name HN  ))
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  (( segid "BrD " and resid 79   and name HB2 ))
ASSI {10471}
  (( segid "BrD " and resid 96   and name HN  ))
  (( segid "BrD " and resid 94   and name HA  ))
    3 900     3.800     1.600 peak 10471 weight  0.10000E+01 volume  0 52287E+02 ppm1      7 984 ppm2      4 814
OR {10471}
  (( segid "BrD " and resid 96   and name HN  ))
  (( segid "BrD " and resid 86   and name HA  ))
OR {10471}
  (( segid "BrD " and resid 96   and name HN  ))
  (( segid "BrD " and resid 92   and name HA  ))
ASSI {10501}
  (( segid "BrD " and resid 80   and name HN  ))
  (( segid "BrD " and resid 80   and name HA  ))
    2 800     2 000     2 000 peak 10501 weight  0.10000E+01 volume  0 42726E+03 ppm1      7 974 ppm2      4 691
OR {10501}
  (( segid "BrD " and resid 80   and name HN  ))
  (( segid "BrD " and resid 76   and name HA  ))
ASSI {10541}
  (( segid "BrD " and resid 55   and name HN  ))
  (  segid "BrD " and resid 58   and name HG2%)
    3 500     3 100     2 000 peak 10541 weight  0 10000E+01 volume  0 11084E+03 ppm1      7 974 ppm2      1 670
OR {10541}
  (( segid "BrD " and resid 78   and name HN  ))
  (  segid "BrD " and resid 22   and name HD1%)
OR {10541}
  (( segid "BrD " and resid 78   and name HN  ))
  (( segid "BrD " and resid 110  and name HG12))
OR {10541}
  (( segid "BrD " and resid 55   and name HN  ))
  (  segid "BrD " and resid 43   and name HB% )
OR {10541}
  (( segid "BrD " and resid 78   and name HN  ))
  (  segid "BrD " and resid 25   and name HG2%)
OR {10541}
  (( segid "BrD " and resid 55   and name HN  ))
  (  segid "BrD " and resid 25   and name HG2%)
OR {10541}
  (( segid "BrD " and resid 78   and name HN  ))
  (  segid "BrD " and resid 63   and name HD1%)
OR {10541}
  (( segid "BrD " and resid 55   and name HN  ))
  (  segid "BrD " and resid 22   and name HD1%)
ASSI {10551}
  (( segid "BrD " and resid 78   and name HN  ))
  (( segid "BrD " and resid 78   and name HB2 ))
    3 400     2.900     2 100 peak 10551 weight  0 10000E+01 volume  0 13253E+03 ppm1      7 975 ppm2      1 068
OR {10551}
  (( segid "BrD " and resid 80   and name HN  ))
  (  segid "BrD " and resid 81   and name HG1%)
OR {10551}
  (( segid "BrD " and resid 78   and name HN  ))
  (  segid "BrD " and resid 81   and name HG1%)
OR {10551}
  (( segid "BrD " and resid 55   and name HN  ))
  (  segid "BrD " and resid 81   and name HG1%)
ASSI {10611}
  (( segid "BrD " and resid 56   and name HN  ))
  (( segid "BrD " and resid 34   and name HB2 ))
    3 100     2 400     2 400 peak 10611 weight  0 10000E+01 volume  0 21458E+03 ppm1      9 680 ppm2      3 118
OR {10611}
  (( segid "BrD " and resid 56   and name HN  ))
  (( segid "BrD " and resid 59   and name HG2 ))
ASSI {10631}
  (( segid "BrD " and resid 82   and name HN  ))
  (  segid "BrD " and resid 83   and name HG2%)
    3 500     3 100     2.000 peak 10631 weight  0 10000E+01 volume  0 97408E+02 ppm1      6 981 ppm2      1 909
OR {10631}
  (( segid "BrD " and resid 82   and name HN  ))
  (( segid "BrD " and resid 103  and name HB2 ))
ASSI {10781}
  (( segid "BrD " and resid 80   and name HN  ))
  (  segid "BrD " and resid 83   and name HG2%)
    3 900     3 800     1 600 peak 10781 weight  0 10000E+01 volume  0 57791E+02 ppm1      8.006 ppm2      1 932
OR {10781}
  (( segid "BrD " and resid 80   and name HN  ))
  (( segid "BrD " and resid 116  and name HG11))
OR {10781}
  (( segid "BrD " and resid 80   and name HN  ))
  (( segid "BrD " and resid 54   and name HB2 ))
ASSI {10811}
  (( segid "BrD " and resid 80   and name HN  ))
  (  segid "BrD " and resid 81   and name HG1%)
    3 600     3 200     1 900 peak 10811 weight  0 10000E+01 volume  0 94805E+02 ppm1      8.005 ppm2      1.064
OR {10811}
  (( segid "BrD " and resid 80   and name HN  ))
  (( segid "BrD " and resid 78   and name HB2 ))
ASSI {10901}
  (( segid "BrD " and resid 85   and name HN  ))
  (( segid "BrD " and resid 86   and name HG1 ))
    3 800     3.600     1 700 peak 10901 weight  0 10000E+01 volume  0.64876E+02 ppm1      7 516 ppm2      1 905
OR {10901}
  (( segid "BrD " and resid 85   and name HN  ))
  (  segid "BrD " and resid 83   and name HG2%)
ASSI {10981}
  (( segid "BrD " and resid 87   and name HN  ))
  (( segid "BrD " and resid 85   and name HA  ))
    3.900     3 800     1 600 peak 10981 weight  0 10000E+01 volume  0 57856E+02 ppm1      8 572 ppm2      5 005
OR {10981}
  (( segid "BrD " and resid 87   and name HN  ))
  (( segid "BrD " and resid 88   and name HA  ))
ASSI {10991}
  (( segid "BrD " and resid 87   and name HN  ))
  (( segid "BrD " and resid 85   and name HB2 ))
    3 200     2.600     2 300 peak 10991 weight  0 10000E+01 volume  0 17351E+03 ppm1      8 571 ppm2      3 639
OR {10991}
  (( segid "BrD " and resid 87   and name HN  ))
  (( segid "BrD " and resid 95   and name HB1 ))
ASSI {11181}
  (( segid "BrD " and resid 93   and name HN  ))
  (( segid "BrD " and resid 91   and name HB1 ))
    3 000     2.200     2 200 peak 11181 weight  0 10000E+01 volume  0 28245E+03 ppm1      8 714 ppm2      3 075
OR {11181}
  (( segid "BrD " and resid 93   and name HN  ))
  (( segid "BrD " and resid 96   and name HB2 ))
ASSI {11231}
  (( segid "BrD " and resid 31   and name HN  ))
  (( segid "BrD " and resid 98   and name HB1 ))
    3 900     3 800     1 600 peak 11231 weight  0 10000E+01 volume  0 56370E+02 ppm1      8 481 ppm2      3 992
OR {11231}
  (( segid "BrD " and resid 31   and name HN  ))
  (( segid "BrD " and resid 32   and name HB2 ))
ASSI {11271}
  (( segid "BrD " and resid 31   and name HN  ))
  (( segid "BrD " and resid 33   and name HD1 ))
    4 100     4 100     1 400 peak 11271 weight  0 10000E+01 volume  0 42900E+02 ppm1      8 480 ppm2      2 781
OR {11271}
  (( segid "BrD " and resid 59   and name HN  ))
  (( segid "BrD " and resid 61   and name HG2 ))
ASSI {11301}
  (( segid "BrD " and resid 31   and name HN  ))
  (  segid "BrD " and resid 101  and name HD1%)
    3.800     3 600     1 700 peak 11301 weight  0.10000E+01 volume  0 60718E+02 ppm1      8 479 ppm2      1 542
OR {11301}
  (( segid "BrD " and resid 31   and name HN  ))
  (  segid "BrD " and resid 56   and name HD1%)
ASSI {11321}
  (( segid "BrD " and resid 59   and name HN  ))
  (  segid "BrD " and resid 81   and name HG1%)
    4 200     4 200     1 300 peak 11321 weight  0 10000E+01 volume  0 33324E+02 ppm1      8.480 ppm2      1 110
OR {11321}
  (( segid "BrD " and resid 31   and name HN  ))
  (( segid "BrD " and resid 33   and name HB1 ))
ASSI {11531}
  (( segid "BrD " and resid 104  and name HN  ))
  (  segid "BrD " and resid 102  and name HD2%)
    4.700     4.700     0 800 peak 11531 weight  0.10000E+01 volume  0 18001E+02 ppm1      7 735 ppm2      1 282
OR {11531}
  (( segid "BrD " and resid 35   and name HN  ))
  (  segid "BrD " and resid 102  and name HD1%)
OR {11531}
  (( segid "BrD " and resid 104  and name HN  ))
  (  segid "BrD " and resid 102  and name HD1%)
ASSI {11541}
  (( segid "BrD " and resid 35   and name HN  ))
  (( segid "BrD " and resid 32   and name HB2 ))
    3 400     2 900     2 100 peak 11541 weight  0 10000E+01 volume  0 13237E+03 ppm1      7 734 ppm2      3 923
OR {11541}
  (( segid "BrD " and resid 104  and name HN  ))
  (( segid "BrD " and resid 106  and name HB1 ))
ASSI {11591}
  (( segid "BrD " and resid 66   and name HN  ))
  (( segid "BrD " and resid 69   and name HB  ))
    3 600     3 200     1 900 peak 11591 weight  0 10000E+01 volume  0.90637E+02 ppm1      8 764 ppm2      2 935
OR {11591}
  (( segid "BrD " and resid 66   and name HN  ))
  (( segid "BrD " and resid 63   and name HB1 ))
ASSI {11631}
  (( segid "BrD " and resid 67   and name HN  ))
  (  segid "BrD " and resid 63   and name HD1%)
    3.500     3.100     2 000 peak 11631 weight  0 10000E+01 volume  0 95713E+02 ppm1      8.632 ppm2      1 678
OR {11631}
  (( segid "BrD " and resid 67   and name HN  ))
  (( segid "BrD " and resid 62   and name HB2 ))
ASSI {11671}
  (( segid "BrD " and resid 68   and name HN  ))
  (  segid "BrD " and resid 63   and name HD1%)
    3.600     3.200     1 900 peak 11671 weight  0 10000E+01 volume  0 92729E+02 ppm1      8 626 ppm2      1.684
OR {11671}
  (( segid "BrD " and resid 68   and name HN  ))
  (( segid "BrD " and resid 62   and name HB2 ))
ASSI {11701}
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   (( segid "BrD " and resid 69   and name HN ))
   (( segid "BrD " and resid 63   and name HG ))
     3 400     2 900     2 100 peak 11701 weight  0 10000E+01 volume  0.12326E+03 ppm1      8 306 ppm2      2 476
OR {11701}
   (( segid "BrD " and resid 69   and name HN ))
   (( segid "BrD " and resid 73   and name HB2 ))
ASSI {11711}
   (( segid "BrD " and resid 69   and name HN ))
   (( segid "BrD " and resid 66   and name HB2 ))
     3 800     3.600     1 700 peak 11711 weight  0.10000E+01 volume  0 68030E+02 ppm1      8 306 ppm2      2 614
OR {11711}
   (( segid "BrD " and resid 69   and name HN ))
   (( segid "BrD " and resid 11   and name HB2 ))
OR {11711}
   (( segid "BrD " and resid 69   and name HN ))
   (( segid "BrD " and resid 73   and name HB1 ))
ASSI {11751}
   (( segid "BrD " and resid 70   and name HN ))
   (( segid "BrD " and resid 73   and name HG ))
     4 200     4 200     1 300 peak 11751 weight  0 10000E+01 volume  0 36902E+02 ppm1      8.039 ppm2      2 374
OR {11751}
   (( segid "BrD " and resid 70   and name HN ))
   (( segid "BrD " and resid 9    and name HB2 ))
ASSI {11761}
   (( segid "BrD " and resid 70   and name HN ))
   (( segid "BrD " and resid 73   and name HB1 ))
     3.500     3 100     2 000 peak 11761 weight  0 10000E+01 volume  0 95470E+02 ppm1      8 040 ppm2      2 594
OR {11761}
   (( segid "BrD " and resid 70   and name HN ))
   (( segid "BrD " and resid 11   and name HB2 ))
ASSI {11851}
   (( segid "BrD " and resid 73   and name HN ))
   (( segid "BrD " and resid 74   and name HB1 ))
     3 600     3 200     1 900 peak 11851 weight  0 10000E+01 volume  0 82682E+02 ppm1      8 045 ppm2      3 572
OR {11851}
   (( segid "BrD " and resid 73   and name HN ))
   (( segid "BrD " and resid 75   and name HG1 ))
ASSI {11931}
   (( segid "BrD " and resid 23   and name HN ))
   (( segid "BrD " and resid 22   and name HA ))
     3 800     3 600     1 700 peak 11931 weight  0.10000E+01 volume  0 64947E+02 ppm1      9 125 ppm2      4 688
OR {11931}
   (( segid "BrD " and resid 75   and name HN ))
   (( segid "BrD " and resid 72   and name HA ))
ASSI {11941}
   (( segid "BrD " and resid 98   and name HN ))
   (( segid "BrD " and resid 100  and name HB2 ))
     4.000     4 000     1 500 peak 11941 weight  0 10000E+01 volume  0 47235E+02 ppm1      9 125 ppm2      3 411
OR {11941}
   (( segid "BrD " and resid 23   and name HN ))
   (( segid "BrD " and resid 24   and name HG1 ))
ASSI {12011}
   (( segid "BrD " and resid 23   and name HN ))
   (  segid "BrD " and resid 22   and name HD2% )
     3.800     3 600     1 700 peak 12011 weight  0 10000E+01 volume  0.60527E+02 ppm1      9 125 ppm2      1 594
OR {12011}
   (( segid "BrD " and resid 23   and name HN ))
   (  segid "BrD " and resid 21   and name HG2% )
ASSI {12021}
   (( segid "BrD " and resid 98   and name HN ))
   (( segid "BrD " and resid 30   and name HB1 ))
     4 000     4.000     1 500 peak 12021 weight  0 10000E+01 volume  0 46966E+02 ppm1      9 124 ppm2      4 936
OR {12021}
   (( segid "BrD " and resid 23   and name HN ))
   (( segid "BrD " and resid 60   and name HB1 ))
OR {12021}
   (( segid "BrD " and resid 98   and name HN ))
   (( segid "BrD " and resid 100  and name HA ))
OR {12021}
   (( segid "BrD " and resid 23   and name HN ))
   (( segid "BrD " and resid 64   and name HA ))
ASSI {12071}
   (( segid "BrD " and resid 100  and name HN ))
   (( segid "BrD " and resid 98   and name HB2 ))
     4 100     4 100     1 400 peak 12071 weight  0 10000E+01 volume  0 37827E+02 ppm1      8 669 ppm2      3 641
OR {12071}
   (( segid "BrD " and resid 100  and name HN ))
   (( segid "BrD " and resid 85   and name HB2 ))
ASSI {12101}
   (( segid "BrD " and resid 100  and name HN ))
   (( segid "BrD " and resid 103  and name HB1 ))
     2 000     2 000     2 500 peak 12101 weight  0 10000E+01 volume  0 26537E+04 ppm1      8 669 ppm2      2 323
OR {12101}
   (( segid "BrD " and resid 100  and name HN ))
   (( segid "BrD " and resid 104  and name HD1 ))
ASSI {12111}
   (( segid "BrD " and resid 100  and name HN ))
   (( segid "BrD " and resid 103  and name HB2 ))
     4 100     4.100     1 400 peak 12111 weight  0.10000E+01 volume  0 37921E+02 ppm1      8.669 ppm2      1 892
OR {12111}
   (( segid "BrD " and resid 100  and name HN ))
   (( segid "BrD " and resid 86   and name HG1 ))
ASSI {12141}
   (( segid "BrD " and resid 100  and name HN ))
   (  segid "BrD " and resid 96   and name HD% )
     4 300     4.300     1 200 peak 12141 weight  0.10000E+01 volume  0 30609E+02 ppm1      8.669 ppm2      7.737
OR {12141}
   (( segid "BrD " and resid 100  and name HN ))
   (( segid "BrD " and resid 104  and name HN ))
ASSI {12251}
   (( segid "BrD " and resid 107  and name HN ))
   (( segid "BrD " and resid 110  and name HB ))
     3 700     3.400     1.800 peak 12251 weight  0 10000E+01 volume  0 79191E+02 ppm1      8.980 ppm2      2.348
OR {12251}
   (( segid "BrD " and resid 107  and name HN ))
   (( segid "BrD " and resid 103  and name HB1 ))
OR {12251}
   (( segid "BrD " and resid 107  and name HN ))
   (( segid "BrD " and resid 109  and name HB1 ))
ASSI {12261}
   (( segid "BrD " and resid 107  and name HN ))
   (( segid "BrD " and resid 102  and name HB2 ))
     5.500     5.500     0.000 peak 12261 weight  0 10000E+01 volume  0 35919E+00 ppm1      8 980 ppm2      1 797
OR {12261}
   (( segid "BrD " and resid 107  and name HN ))
   (  segid "BrD " and resid 25   and name HG1% )
ASSI {12281}
   (( segid "BrD " and resid 108  and name HN ))
   (( segid "BrD " and resid 103  and name HG2 ))
     4 100     4 100     1 400 peak 12281 weight  0 10000E+01 volume  0 42059E+02 ppm1      8 522 ppm2      2 529
OR {12281}
   (( segid "BrD " and resid 108  and name HN ))
   (( segid "BrD " and resid 104  and name HB1 ))
ASSI {12301}
   (( segid "BrD " and resid 108  and name HN ))
   (  segid "BrD " and resid 116  and name HD1% )
     3 900     3.800     1 600 peak 12301 weight  0 10000E+01 volume  0 52230E+02 ppm1      8 521 ppm2      1 422
OR {12301}
   (( segid "BrD " and resid 108  and name HN ))
   (( segid "BrD " and resid 109  and name HG1 ))
ASSI {12311}
   (( segid "BrD " and resid 108  and name HN ))
   (( segid "BrD " and resid 110  and name HB ))
     4 100     4 100     1 400 peak 12311 weight  0 10000E+01 volume  0 41867E+02 ppm1      8 522 ppm2      2 331
OR {12311}
   (( segid "BrD " and resid 108  and name HN ))
   (( segid "BrD " and resid 109  and name HB1 ))
ASSI {12401}
   (( segid "BrD " and resid 113  and name HN ))
   (( segid "BrD " and resid 115  and name HG ))
     3 300     2.700     2 200 peak 12401 weight  0 10000E+01 volume  0 16014E+03 ppm1      8 218 ppm2      2 152
OR {12401}
   (( segid "BrD " and resid 113  and name HN ))
   (( segid "BrD " and resid 115  and name HB1 ))
OR {12401}
   (( segid "BrD " and resid 113  and name HN ))
   (( segid "BrD " and resid 109  and name HB2 ))
ASSI {12501}
   (( segid "BrD " and resid 116  and name HN ))
   (( segid "BrD " and resid 71   and name HA ))
     4 300     4 300     1 200 peak 12501 weight  0 10000E+01 volume  0.28782E+02 ppm1      8 087 ppm2      4.664
OR {12501}
   (( segid "BrD " and resid 116  and name HN ))
   (( segid "BrD " and resid 72   and name HA ))
OR {12501}
   (( segid "BrD " and resid 116  and name HN ))
   (( segid "BrD " and resid 114  and name HA1 ))
OR {12501}
   (( segid "BrD " and resid 116  and name HN ))
   (( segid "BrD " and resid 76   and name HA ))
ASSI {12511}
   (( segid "BrD " and resid 116  and name HN ))
   (( segid "BrD " and resid 75   and name HA ))
     3.600     3 200     1 900 peak 12511 weight  0 10000E+01 volume  0 81005E+02 ppm1      8 087 ppm2      4 526
OR {12511}
   (( segid "BrD " and resid 116  and name HN ))
   (( segid "BrD " and resid 114  and name HA2 ))
ASSI {12601}
   (( segid "BrD " and resid 92   and name HN ))
   (( segid "BrD " and resid 92   and name HB1 ))
     4 100     4 100     1 400 peak 12601 weight  0 10000E+01 volume  0 37922E+02 ppm1      8 831 ppm2      2.695
OR {12601}
   (( segid "BrD " and resid 92   and name HN ))
   (( segid "BrD " and resid 91   and name HB2 ))
ASSI {12841}
   (( segid "BrD " and resid 19   and name HN ))
   (( segid "BrD " and resid 17   and name HB ))
     3.800     3 600     1 700 peak 12841 weight  0 10000E+01 volume  0 59211E+02 ppm1      9.187 ppm2      4 880
OR {12841}
   (( segid "BrD " and resid 19   and name HN ))
   (( segid "BrD " and resid 20   and name HA ))
ASSI {12861}
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   (( segid "BrD " and resid 20   and name HN  ))
   (( segid "BrD " and resid 63   and name HG  ))
     4 000     4 000     1 500 peak 12861 weight  0 10000E+01 volume  0 43415E+02 ppm1      8 147 ppm2      2 471
OR (12861)
   (( segid "BrD " and resid 20   and name HN  ))
   (( segid "BrD " and resid 21   and name HB  ))
ASSI (12951)
   (( segid "BrD " and resid 23   and name HN  ))
   (  segid "BrD " and resid 25   and name HG1%)
     3 800     3 600     1 700 peak 12951 weight  0.10000E+01 volume  0.65898E+02 ppm1      9 119 ppm2      1.823
OR (12951)
   (( segid "BrD " and resid 98   and name HN  ))
   (( segid "BrD " and resid 101  and name HG12))
ASSI (12961)
   (( segid "BrD " and resid 23   and name HN  ))
   (  segid "BrD " and resid 22   and name HD1%)
     3 100     2 400     2 400 peak 12961 weight  0 10000E+01 volume  0 23452E+03 ppm1      9 120 ppm2      1.646
OR (12961)
   (( segid "BrD " and resid 23   and name HN  ))
   (( segid "BrD " and resid 21   and name HG12))
OR (12961)
   (( segid "BrD " and resid 23   and name HN  ))
   (  segid "BrD " and resid 21   and name HG2%)
OR (12961)
   (( segid "BrD " and resid 23   and name HN  ))
   (  segid "BrD " and resid 25   and name HG2%)
ASSI (12971)
   (( segid "BrD " and resid 98   and name HN  ))
   (  segid "BrD " and resid 101  and name HD1%)
     3 900     3 800     1 600 peak 12971 weight  0 10000E+01 volume  0 50522E+02 ppm1      9 119 ppm2      1 514
OR (12971)
   (( segid "BrD " and resid 23   and name HN  ))
   (  segid "BrD " and resid 63   and name HD2%)
ASSI (12981)
   (( segid "BrD " and resid 98   and name HN  ))
   (( segid "BrD " and resid 100  and name HB2 ))
     3.400     2 900     2 100 peak 12981 weight  0 10000E+01 volume  0 12055E+03 ppm1      9 119 ppm2      3 467
OR (12981)
   (( segid "BrD " and resid 23   and name HN  ))
   (( segid "BrD " and resid 24   and name HG1 ))
OR (12981)
   (( segid "BrD " and resid 98   and name HN  ))
   (( segid "BrD " and resid 100  and name HB1 ))
ASSI (13001)
   (( segid "BrD " and resid 98   and name HN  ))
   (  segid "BrD " and resid 95   and name HD% )
     3 900     3.800     1 600 peak 13001 weight  0 10000E+01 volume  0 54095E+02 ppm1      9 119 ppm2      7 520
OR (13001)
   (( segid "BrD " and resid 23   and name HN  ))
   (( segid "BrD " and resid 24   and name HE22))
OR (13001)
   (( segid "BrD " and resid 23   and name HN  ))
   (  segid "BrD " and resid 74   and name HE% )
ASSI (13011)
   (( segid "BrD " and resid 26   and name HN  ))
   (  segid "BrD " and resid 31   and name HB% )
     3 500     3 100     2 000 peak 13011 weight  0 10000E+01 volume  0 10060E+03 ppm1      9 196 ppm2      2 308
OR (13011)
   (( segid "BrD " and resid 26   and name HN  ))
   (( segid "BrD " and resid 22   and name HB2 ))
ASSI (13121)
   (( segid "BrD " and resid 59   and name HN  ))
   (( segid "BrD " and resid 56   and name HB2 ))
     3 800     3 600     1.700 peak 13121 weight  0 10000E+01 volume  0 59266E+02 ppm1      8 496 ppm2      2 008
OR (13121)
   (( segid "BrD " and resid 59   and name HN  ))
   (( segid "BrD " and resid 57   and name HG2 ))
OR (13121)
   (( segid "BrD " and resid 31   and name HN  ))
   (( segid "BrD " and resid 102  and name HB1 ))
ASSI (13171)
   (( segid "BrD " and resid 60   and name HN  ))
   (( segid "BrD " and resid 57   and name HB2 ))
     3 500     3 100     2 000 peak 13171 weight  0 10000E+01 volume  0 10295E+03 ppm1      8 564 ppm2      2 858
OR (13171)
   (( segid "BrD " and resid 60   and name HN  ))
   (( segid "BrD " and resid 61   and name HB1 ))
OR (13171)
   (( segid "BrD " and resid 65   and name HN  ))
   (( segid "BrD " and resid 61   and name HB1 ))
ASSI (13181)
   (( segid "BrD " and resid 60   and name HN  ))
   (( segid "BrD " and resid 22   and name HG  ))
     3 800     3 600     1.700 peak 13181 weight  0 10000E+01 volume  0 61364E+02 ppm1      8 565 ppm2      2.336
OR (13181)
   (( segid "BrD " and resid 65   and name HN  ))
   (( segid "BrD " and resid 62   and name HG1 ))
OR (13181)
   (( segid "BrD " and resid 60   and name HN  ))
   (( segid "BrD " and resid 56   and name HG  ))
OR (13181)
   (( segid "BrD " and resid 60   and name HN  ))
   (( segid "BrD " and resid 22   and name HB2 ))
OR (13181)
   (( segid "BrD " and resid 60   and name HN  ))
   (( segid "BrD " and resid 57   and name HD2 ))
ASSI (13191)
   (( segid "BrD " and resid 60   and name HN  ))
   (  segid "BrD " and resid 22   and name HD1%)
     3 200     2.600     2 300 peak 13191 weight  0.10000E+01 volume  0 17809E+03 ppm1      8 568 ppm2      1.666
OR (13191)
   (( segid "BrD " and resid 65   and name HN  ))
   (  segid "BrD " and resid 63   and name HD1%)
OR (13191)
   (( segid "BrD " and resid 60   and name HN  ))
   (  segid "BrD " and resid 58   and name HG2%)
ASSI (13201)
   (( segid "BrD " and resid 65   and name HN  ))
   (  segid "BrD " and resid 63   and name HD2%)
     3 600     3.200     1 900 peak 13201 weight  0 10000E+01 volume  0.81304E+02 ppm1      8 565 ppm2      1 497
OR (13201)
   (( segid "BrD " and resid 65   and name HN  ))
   (( segid "BrD " and resid 62   and name HG2 ))
OR (13201)
   (( segid "BrD " and resid 60   and name HN  ))
   (  segid "BrD " and resid 63   and name HD2%)
ASSI (13631)
   (( segid "BrD " and resid 84   and name HN  ))
   (( segid "BrD " and resid 82   and name HN  ))
     4.000     4 000     1 500 peak 13631 weight  0 10000E+01 volume  0 44090E+02 ppm1      9 463 ppm2      6.981
OR (13631)
   (( segid "BrD " and resid 63   and name HN  ))
   (  segid "BrD " and resid 74   and name HD% )
ASSI (13691)
   (( segid "BrD " and resid 22   and name HN  ))
   (( segid "BrD " and resid 22   and name HB2 ))
     3 700     3 400     1 800 peak 13691 weight  0 10000E+01 volume  0 68908E+02 ppm1      9 473 ppm2      2 333
OR (13691)
   (( segid "BrD " and resid 22   and name HN  ))
   (( segid "BrD " and resid 21   and name HG11))
OR (13691)
   (( segid "BrD " and resid 22   and name HN  ))
   (( segid "BrD " and resid 22   and name HG  ))
ASSI (13971)
   (( segid "BrD " and resid 114  and name HN  ))
   (( segid "BrD " and resid 112  and name HG2 ))
     4 900     4 900     0 600 peak 13971 weight  0.10000E+01 volume  0 14459E+02 ppm1      8 377 ppm2      2.786
OR (13971)
   (( segid "BrD " and resid 114  and name HN  ))
   (( segid "BrD " and resid 13   and name HB1 ))
ASSI (14061)
   (( segid "BrD " and resid 107  and name HN  ))
   (  segid "BrD " and resid 110  and name HG2%)
     4.800     4 800     0 700 peak 14061 weight  0 10000E+01 volume  0 15271E+02 ppm1      8 980 ppm2      1 260
OR (14061)
   (( segid "BrD " and resid 107  and name HN  ))
   (  segid "BrD " and resid 21   and name HD1%)
ASSI (14071)
   (( segid "BrD " and resid 106  and name HN  ))
   (( segid "BrD " and resid 107  and name HA  ))
     4 600     4 600     0 900 peak 14071 weight  0 10000E+01 volume  0 20679E+02 ppm1      9.742 ppm2      4.447
OR (14071)
   (( segid "BrD " and resid 106  and name HN  ))
   (( segid "BrD " and resid 99   and name HA  ))
ASSI (14131)
   (( segid "BrD " and resid 104  and name HN  ))
   (( segid "BrD " and resid 102  and name HB2 ))
     3.700     3 400     1 800 peak 14131 weight  0 10000E+01 volume  0 79648E+02 ppm1      7 763 ppm2      1 816
OR (14131)
   (( segid "BrD " and resid 104  and name HN  ))
   (( segid "BrD " and resid 101  and name HG12))
ASSI (14141)
   (( segid "BrD " and resid 103  and name HN  ))
   (( segid "BrD " and resid 106  and name HB1 ))
     3.600     3 200     1 900 peak 14141 weight  0 10000E+01 volume  0 92105E+02 ppm1      8 695 ppm2      3 908
OR (14141)
   (( segid "BrD " and resid 17   and name HN  ))
   (( segid "BrD " and resid 18   and name HA  ))
ASSI (14151)
   (( segid "BrD " and resid 102  and name HN  ))
   (( segid "BrD " and resid 105  and name HB2 ))
     4 000     4 000     1 500 peak 14151 weight  0 10000E+01 volume  0 49406E+02 ppm1      9.156 ppm2      3.635
OR (14151)
   (( segid "BrD " and resid 102  and name HN  ))
   (( segid "BrD " and resid 98   and name HB2 ))
OR (14151)
   (( segid "BrD " and resid 102  and name HN  ))
   (( segid "BrD " and resid 106  and name HB2 ))
ASSI (14161)
   (( segid "BrD " and resid 102  and name HN  ))
   (( segid "BrD " and resid 103  and name HA  ))
     5.000     5 000     0 500 peak 14161 weight  0 10000E+01 volume  0 12711E+02 ppm1      9 156 ppm2      3 753
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OR (14161)
  (( segid "BrD " and resid 102  and name HN  ))
  (( segid "BrD " and resid 105  and name HB1 ))
ASSI (14171)
  (( segid "BrD " and resid 101  and name HN  ))
  (( segid "BrD " and resid 104  and name HN  ))
    4 300     4 300     1 200 peak 14171 weight  0 10000E+01 volume  0 29353E+02 ppm1      8 513 ppm2      7 761
OR (14171)
  (( segid "BrD " and resid 101  and name HN  ))
  (  segid "BrD " and resid 34   and name HE% )
ASSI (14201)
  (( segid "BrD " and resid 100  and name HN  ))
  (( segid "BrD " and resid 86   and name HE1 ))
    4.100     4 100     1 400 peak 14201 weight  0 10000E+01 volume  0 38990E+02 ppm1      8.667 ppm2      3 092
OR (14201)
  (( segid "BrD " and resid 100  and name HN  ))
  (( segid "BrD " and resid 96   and name HB2 ))
ASSI (14221)
  (( segid "BrD " and resid 100  and name HN  ))
  (( segid "BrD " and resid 101  and name HG12))
    4 800     4 800     0 700 peak 14221 weight  0 10000E+01 volume  0 14931E+02 ppm1      8.669 ppm2      1 806
OR (14221)
  (( segid "BrD " and resid 100  and name HN  ))
  (( segid "BrD " and resid 102  and name HB2 ))
ASSI (14241)
  (( segid "BrD " and resid 99   and name HN  ))
  (( segid "BrD " and resid 96   and name HB2 ))
    4 900     4 900     0 600 peak 14241 weight  0 10000E+01 volume  0 14325E+02 ppm1      8 940 ppm2      3 103
OR (14241)
  (( segid "BrD " and resid 99   and name HN  ))
  (( segid "BrD " and resid 94   and name HG1 ))
OR (14241)
  (( segid "BrD " and resid 99   and name HN  ))
  (( segid "BrD " and resid 86   and name HE1 ))
ASSI (14251)
  (( segid "BrD " and resid 99   and name HN  ))
  (  segid "BrD " and resid 81   and name HG2% )
    5 500     5 500     0 000 peak 14251 weight  0 10000E+01 volume  0 30696E+01 ppm1      8 934 ppm2      0 748
OR (14251)
  (( segid "BrD " and resid 99   and name HN  ))
  (( segid "BrD " and resid 86   and name HG2 ))
ASSI (14281)
  (( segid "BrD " and resid 98   and name HN  ))
  (( segid "BrD " and resid 32   and name HH2 ))
    3 800     3 600     1 700 peak 14281 weight  0.10000E+01 volume  0 66237E+02 ppm1      9 125 ppm2      7 750
OR (14281)
  (( segid "BrD " and resid 98   and name HN  ))
  (  segid "BrD " and resid 34   and name HE% )
OR (14281)
  (( segid "BrD " and resid 75   and name HN  ))
  (  segid "BrD " and resid 68   and name HD% )
ASSI (14301)
  (( segid "BrD " and resid 96   and name HN  ))
  (  segid "BrD " and resid 99   and name HB% )
    3 600     3 200     1 900 peak 14301 weight  0 10000E+01 volume  0 84940E+02 ppm1      7 977 ppm2      2 199
OR (14301)
  (( segid "BrD " and resid 96   and name HN  ))
  (( segid "BrD " and resid 97   and name HG2 ))
ASSI (14311)
  (( segid "BrD " and resid 77   and name HN  ))
  (  segid "BrD " and resid 73   and name HD1% )
    4 900     4 900     0.600 peak 14311 weight  0.10000E+01 volume  0.13346E+02 ppm1      7 981 ppm2      1 543
OR (14311)
  (( segid "BrD " and resid 78   and name HN  ))
  (( segid "BrD " and resid 116  and name HG12))
OR (14311)
  (( segid "BrD " and resid 78   and name HN  ))
  (  segid "BrD " and resid 56   and name HD1% )
OR (14311)
  (( segid "BrD " and resid 77   and name HN  ))
  (( segid "BrD " and resid 116  and name HG12))
OR (14311)
  (( segid "BrD " and resid 96   and name HN  ))
  (  segid "BrD " and resid 101  and name HD1% )
ASSI (14441)
  (( segid "BrD " and resid 83   and name HN  ))
  (( segid "BrD " and resid 79   and name HG1 ))
    4 600     4 600     0 900 peak 14441 weight  0 10000E+01 volume  0 19968E+02 ppm1      9 658 ppm2      3 046
OR (14441)
  (( segid "BrD " and resid 83   and name HN  ))
  (( segid "BrD " and resid 87   and name HG1 ))
ASSI (14451)
  (( segid "BrD " and resid 83   and name HN  ))
  (( segid "BrD " and resid 80   and name HG1 ))
    5 500     5.500     0.000 peak 14451 weight  0 10000E+01 volume  0 45437E+00 ppm1      9 658 ppm2      2 374
OR (14451)
  (( segid "BrD " and resid 83   and name HN  ))
  (( segid "BrD " and resid 86   and name HB1 ))
ASSI (14461)
  (( segid "BrD " and resid 83   and name HN  ))
  (( segid "BrD " and resid 86   and name HG2 ))
    5.000     5.000     0.500 peak 14461 weight  0.10000E+01 volume  0.12633E+02 ppm1      9.657 ppm2      0 743
OR (14461)
  (( segid "BrD " and resid 83   and name HN  ))
  (  segid "BrD " and resid 81   and name HG2% )
ASSI (14511)
  (( segid "BrD " and resid 79   and name HN  ))
  (  segid "BrD " and resid 106  and name HE% )
    3 600     3 200     1 900 peak 14511 weight  0 10000E+01 volume  0 86513E+02 ppm1      8 680 ppm2      7 621
OR (14511)
  (( segid "BrD " and resid 79   and name HN  ))
  (( segid "BrD " and resid 81   and name HN  ))
ASSI (14591)
  (( segid "BrD " and resid 72   and name HN  ))
  (( segid "BrD " and resid 73   and name HA  ))
    4 100     4 100     1 400 peak 14591 weight  0.10000E+01 volume  0 40514E+02 ppm1      8 858 ppm2      4 801
OR (14591)
  (( segid "BrD " and resid 72   and name HN  ))
  (( segid "BrD " and resid 70   and name HB1 ))
OR (14591)
  (( segid "BrD " and resid 72   and name HN  ))
  (( segid "BrD " and resid 115  and name HA  ))
ASSI (14631)
  (( segid "BrD " and resid 66   and name HN  ))
  (( segid "BrD " and resid 67   and name HA  ))
    4 400     4 400     1 100 peak 14631 weight  0 10000E+01 volume  0.25627E+02 ppm1      8.762 ppm2      4 678
OR (14631)
  (( segid "BrD " and resid 66   and name HN  ))
  (( segid "BrD " and resid 69   and name HA  ))
OR (14631)
  (( segid "BrD " and resid 66   and name HN  ))
  (( segid "BrD " and resid 61   and name HA  ))
ASSI (14641)
  (( segid "BrD " and resid 60   and name HN  ))
  (( segid "BrD " and resid 62   and name HN  ))
    4.200     4 200     1 300 peak 14641 weight  0 10000E+01 volume  0 32935E+02 ppm1      8 568 ppm2      8.968
OR (14641)
  (( segid "BrD " and resid 65   and name HN  ))
  (( segid "BrD " and resid 62   and name HN  ))
ASSI (14651)
  (( segid "BrD " and resid 65   and name HN  ))
  (( segid "BrD " and resid 65   and name HD22))
    4.200     4 200     1 300 peak 14651 weight  0.10000E+01 volume  0 33097E+02 ppm1      8 566 ppm2      7 569
OR (14651)
  (( segid "BrD " and resid 60   and name HN  ))
  (  segid "BrD " and resid 74   and name HE% )
ASSI (14751)
  (( segid "BrD " and resid 62   and name HN  ))
  (( segid "BrD " and resid 64   and name HN  ))
    2 800     2 000     2 000 peak 14751 weight  0 10000E+01 volume  0 39545E+03 ppm1      8 998 ppm2      8 576
OR (14751)
  (( segid "BrD " and resid 62   and name HN  ))
  (( segid "BrD " and resid 60   and name HN  ))
ASSI (14791)
  (( segid "BrD " and resid 38   and name HN  ))
  (( segid "BrD " and resid 37   and name HG2 ))
    3 900     3 800     1.600 peak 14791 weight  0 10000E+01 volume  0.52365E+02 ppm1      8 742 ppm2      2 547
OR (14791)
  (( segid "BrD " and resid 61   and name HN  ))
  (  segid "BrD " and resid 54   and name HE% )
OR (14791)
  (( segid "BrD " and resid 61   and name HN  ))
  (( segid "BrD " and resid 59   and name HB2 ))
OR (14791)
  (( segid "BrD " and resid 61   and name HN  ))
  (( segid "BrD " and resid 63   and name HB2 ))
ASSI (14801)
  (( segid "BrD " and resid 65   and name HN  ))
  (( segid "BrD " and resid 63   and name HN  ))
    4 400     4 400     1 100 peak 14801 weight  0 10000E+01 volume  0 24650E+02 ppm1      8 570 ppm2      9 470
OR (14801)
  (( segid "BrD " and resid 60   and name HN  ))
  (( segid "BrD " and resid 63   and name HN  ))
ASSI (14821)
  (( segid "BrD " and resid 59   and name HN  ))
  (( segid "BrD " and resid 55   and name HN  ))
    3 600     3 200     1 900 peak 14821 weight  0 10000E+01 volume  0 84273E+02 ppm1      8 498 ppm2      7 974
OR (14821)
  (( segid "BrD " and resid 31   and name HN  ))
  (( segid "BrD " and resid 32   and name HE3 ))
ASSI (14901)
  (( segid "BrD " and resid 54   and name HN  ))
  (( segid "BrD " and resid 55   and name HB1 ))
    4 400     4 400     1 100 peak 14901 weight  0.10000E+01 volume  0 25948E+02 ppm1      9 035 ppm2      2 965
OR (14901)
  (( segid "BrD " and resid 54   and name HN  ))
  (( segid "BrD " and resid 37   and name HB1 ))
ASSI (14921)
  (( segid "BrD " and resid 54   and name HN  ))
  (  segid "BrD " and resid 81   and name HG1% )
    4 000     4 000     1 500 peak 14921 weight  0.10000E+01 volume  0.46525E+02 ppm1      9 037 ppm2      1 081
OR (14921)
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  (( segid "BrD " and resid 54   and name HN  ))
  (  segid "BrD " and resid 38   and name HG1%)
ASSI {14931}
  (( segid "BrD " and resid 52   and name HN  ))
  (  segid "BrD " and resid 50   and name HD1%)
     5 500      5 500      0 000 peak 14931 weight  0 10000E+01 volume  0 20319E+01 ppm1      9 004 ppm2      1 110
OR {14931}
  (( segid "BrD " and resid 52   and name HN  ))
  (  segid "BrD " and resid 81   and name HG1%)
ASSI {15021}
  (( segid "BrD " and resid 50   and name HN  ))
  (( segid "BrD " and resid 49   and name HB  ))
     3.400      2 900      2 100 peak 15021 weight  0 10000E+01 volume  0 11615E+03 ppm1      8 562 ppm2      2 642
OR {15021}
  (( segid "BrD " and resid 46   and name HN  ))
  (( segid "BrD " and resid 44   and name HB2 ))
ASSI {15091}
  (( segid "BrD " and resid 35   and name HN  ))
  (( segid "BrD " and resid 33   and name HB1 ))
     5 000      5.000      0 500 peak 15091 weight  0 10000E+01 volume  0 12753E+02 ppm1      7 735 ppm2      1 073
OR {15091}
  (( segid "BrD " and resid 35   and name HN  ))
  (  segid "BrD " and resid 81   and name HG1%)
ASSI {15181}
  (( segid "BrD " and resid 30   and name HN  ))
  (  segid "BrD " and resid 101  and name HG2%)
     3 900      3.800      1 600 peak 15181 weight  0 10000E+01 volume  0 50580E+02 ppm1     12 275 ppm2      1.601
OR {15181}
  (( segid "BrD " and resid 30   and name HN  ))
  (  segid "BrD " and resid 25   and name HG2%)
ASSI {15221}
  (( segid "BrD " and resid 28   and name HN  ))
  (( segid "BrD " and resid 32   and name HN  ))
     4 200      4 200      1 300 peak 15221 weight  0 10000E+01 volume  0 33692E+02 ppm1      8 166 ppm2      7 752
OR {15221}
  (( segid "BrD " and resid 28   and name HN  ))
  (  segid "BrD " and resid 34   and name HE% )
ASSI {15331}
  (( segid "BrD " and resid 25   and name HN  ))
  (  segid "BrD " and resid 31   and name HB% )
     4 500      4 500      1 000 peak 15331 weight  0 10000E+01 volume  0 22185E+02 ppm1      9 133 ppm2      2 295
OR {15331}
  (( segid "BrD " and resid 25   and name HN  ))
  (( segid "BrD " and resid 22   and name HB2 ))
ASSI {15341}
  (( segid "BrD " and resid 24   and name HN  ))
  (( segid "BrD " and resid 27   and name HN  ))
     3 700      3 400      1 800 peak 15341 weight  0 10000E+01 volume  0 78760E+02 ppm1      8 660 ppm2      8 147
OR {15341}
  (( segid "BrD " and resid 24   and name HN  ))
  (( segid "BrD " and resid 20   and name HN  ))
ASSI {15411}
  (( segid "BrD " and resid 18   and name HN  ))
  (( segid "BrD " and resid 21   and name HG12))
     4 300      4.300      1 200 peak 15411 weight  0 10000E+01 volume  0 29441E+02 ppm1      9 077 ppm2      1.642
OR {15411}
  (( segid "BrD " and resid 18   and name HN  ))
  (  segid "BrD " and resid 63   and name HD1%)
OR {15411}
  (( segid "BrD " and resid 18   and name HN  ))
  (  segid "BrD " and resid 21   and name HG2%)
ASSI {15451}
  (( segid "BrD " and resid 17   and name HN  ))
  (  segid "BrD " and resid 15   and name HD% )
     4 700      4 700      0 800 peak 15451 weight  0 10000E+01 volume  0 16799E+02 ppm1      8 669 ppm2      7 656
OR {15451}
  (( segid "BrD " and resid 17   and name HN  ))
  (  segid "BrD " and resid 106  and name HE% )
ASSI {15461}
  (( segid "BrD " and resid 16   and name HN  ))
  (  segid "BrD " and resid 14   and name HD2%)
     4 800      4 800      0 700 peak 15461 weight  0 10000E+01 volume  0 14734E+02 ppm1      8 791 ppm2      1 430
OR {15461}
  (( segid "BrD " and resid 16   and name HN  ))
  (  segid "BrD " and resid 69   and name HG2%)
OR {15461}
  (( segid "BrD " and resid 16   and name HN  ))
  (  segid "BrD " and resid 14   and name HD1%)
ASSI {15491}
  (( segid "BrD " and resid 14   and name HN  ))
  (( segid "BrD " and resid 15   and name HB1 ))
     5 000      5 000      0 500 peak 15491 weight  0 10000E+01 volume  0 11598E+02 ppm1      8 809 ppm2      3.823
OR {15491}
  (( segid "BrD " and resid 13   and name HN  ))
  (( segid "BrD " and resid 15   and name HB1 ))
ASSI {15501}
  (( segid "BrD " and resid 14   and name HN  ))
  (( segid "BrD " and resid 15   and name HB2 ))
     5 100      5 100      0 400 peak 15501 weight  0 10000E+01 volume  0 11421E+02 ppm1      8 809 ppm2      3.641
OR {15501}
  (( segid "BrD " and resid 13   and name HN  ))
  (( segid "BrD " and resid 15   and name HB2 ))
ASSI {15581}
  (( segid "BrD " and resid 32   and name HE1 ))
  (( segid "BrD " and resid 30   and name HB1 ))
     4.800      4.800      0 700 peak 15581 weight  0 10000E+01 volume  0.15339E+02 ppm1     11 082 ppm2      4 955
OR {15581}
  (( segid "BrD " and resid 32   and name HE1 ))
  (( segid "BrD " and resid 32   and name HA  ))
ASSI {15621}
  (( segid "BrD " and resid 32   and name HE1 ))
  (( segid "BrD " and resid 33   and name HD1 ))
     4 200      4 200      1 300 peak 15621 weight  0.10000E+01 volume  0 36353E+02 ppm1     11 082 ppm2      2 779
OR {15621}
  (( segid "BrD " and resid 32   and name HE1 ))
  (( segid "BrD " and resid 94   and name HB1 ))
ASSI {  862}
  (( segid "BrD " and resid 95   and name HB2 ))
  (( segid "BrD " and resid 95   and name HA  ))
     2 900      2 100      2 100 peak  862 weight  0 10000E+01 volume  0 13207E+03 ppm1      3 373 ppm2      4 477
OR {  862}
  (( segid "BrD " and resid 65   and name HB2 ))
  (( segid "BrD " and resid 62   and name HA  ))
ASSI { 5972}
  (  segid "BrD " and resid 18   and name HD1%)
  (( segid "BrD " and resid 68   and name HB1 ))
     2 800      2 000      2 000 peak 5972 weight  0.10000E+01 volume  0 16386E+03 ppm1      1 057 ppm2      3 667
OR { 5972}
  (  segid "BrD " and resid 18   and name HD1%)
  (( segid "BrD " and resid 15   and name HB2 ))
ASSI { 6172}
  (  segid "BrD " and resid 56   and name HD1%)
  (( segid "BrD " and resid 26   and name HA  ))
     3.000      2 200      2.200 peak 6172 weight  0 10000E+01 volume  0 11879E+03 ppm1      1 546 ppm2      4 502
OR { 6172}
  (( segid "BrD " and resid 116  and name HG12))
  (( segid "BrD " and resid 75   and name HA  ))
ASSI { 6592}
  (  segid "BrD " and resid 31   and name HB% )
  (  segid "BrD " and resid 35   and name HE% )
     3 000      2 200      2 200 peak 6592 weight  0.10000E+01 volume  0.12050E+03 ppm1      2 289 ppm2      2 779
OR { 6592}
  (  segid "BrD " and resid 31   and name HB% )
  (( segid "BrD " and resid 33   and name HD1 ))
ASSI { 6622}
  (  segid "BrD " and resid 31   and name HB% )
  (( segid "BrD " and resid 56   and name HB2 ))
     3.200      2 600      2 300 peak 6622 weight  0 10000E+01 volume  0 78528E+02 ppm1      2 291 ppm2      1 994
OR { 6622}
  (  segid "BrD " and resid 31   and name HB% )
  (( segid "BrD " and resid 102  and name HB1 ))
ASSI { 6812}
  (  segid "BrD " and resid 99   and name HB% )
  (( segid "BrD " and resid 85   and name HB2 ))
     2 500      1.600      1 600 peak 6812 weight  0 10000E+01 volume  0.30669E+03 ppm1      2 190 ppm2      3.645
OR { 6812}
  (  segid "BrD " and resid 99   and name HB% )
  (( segid "BrD " and resid 82   and name HB1 ))
ASSI { 6822}
  (  segid "BrD " and resid 99   and name HB% )
  (( segid "BrD " and resid 103  and name HB2 ))
     2.900      2 100      2.100 peak 6822 weight  0 10000E+01 volume  0 12780E+03 ppm1      2 190 ppm2      1 903
OR { 6822}
  (  segid "BrD " and resid 99   and name HB% )
  (( segid "BrD " and resid 86   and name HG1 ))
ASSI { 7132}
  (  segid "BrD " and resid 38   and name HG1%)
  (( segid "BrD " and resid 46   and name HB1 ))
     2 600      1 700      1.700 peak 7132 weight  0 10000E+01 volume  0 23427E+03 ppm1      1 057 ppm2      3 306
OR { 7132}
  (  segid "BrD " and resid 81   and name HG1%)
  (( segid "BrD " and resid 77   and name HB1 ))
ASSI { 7142}
  (  segid "BrD " and resid 81   and name HG1%)
  (( segid "BrD " and resid 59   and name HB2 ))
     2 800      2 000      2.000 peak 7142 weight  0 10000E+01 volume  0.18258E+03 ppm1      1 058 ppm2      2 475
OR { 7142}
  (  segid "BrD " and resid 38   and name HG1%)
  (( segid "BrD " and resid 53   and name HG2 ))
ASSI { 7152}
  (  segid "BrD " and resid 81   and name HG1%)
  (( segid "BrD " and resid 54   and name HB2 ))
     2.800      2 000      2 000 peak 7152 weight  0 10000E+01 volume  0 17360E+03 ppm1      1 057 ppm2      1 962
OR { 7152}
  (  segid "BrD " and resid 81   and name HG1%)
  (( segid "BrD " and resid 56   and name HB2 ))
ASSI { 7222}
  (( segid "BrD " and resid 17   and name HB  ))
  (  segid "BrD " and resid 14   and name HD2%)
     3.200      2.600      2 300 peak 7222 weight  0 10000E+01 volume  0 77701E+02 ppm1      4 854 ppm2      1 424
OR { 7222}
  (( segid "BrD " and resid 17   and name HB  ))
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   ( segid "BrD " and resid 14   and name HD1%)
OR { 7222}
   (( segid "BrD " and resid 17   and name HB  ))
   (( segid "BrD " and resid 109  and name HG1 ))
ASSI { 7232}
   (( segid "BrD " and resid 17   and name HB  ))
   ( segid "BrD " and resid 115  and name HD1%)
     3 400     2 900     2 100 peak  7232 weight  0 10000E+01 volume  0.48663E+02 ppm1      4 854 ppm2      1 377
OR { 7232}
   (( segid "BrD " and resid 17   and name HB  ))
   ( segid "BrD " and resid 14   and name HD2%)
ASSI { 7262}
   ( segid "BrD " and resid 17   and name HG2%)
   ( segid "BrD " and resid 21   and name HD1%)
     2 400     1 400     1 400 peak  7262 weight  0 10000E+01 volume  0 43712E+03 ppm1      1 747 ppm2      1 221
OR { 7262}
   ( segid "BrD " and resid 17   and name HG2%)
   ( segid "BrD " and resid 110  and name HG2%)
ASSI { 7392}
   (( segid "BrD " and resid 15   and name HA  ))
   (( segid "BrD " and resid 18   and name HG  ))
     3 800     3 600     1 700 peak  7392 weight  0 10000E+01 volume  0 25131E+02 ppm1      4 605 ppm2      2 314
OR { 7392}
   (( segid "BrD " and resid 15   and name HA  ))
   (( segid "BrD " and resid 19   and name HB1 ))
ASSI { 7742}
   (( segid "BrD " and resid 106  and name HA  ))
   ( segid "BrD " and resid 25   and name HG1%)
     3 400     2 900     2 100 peak  7742 weight  0 10000E+01 volume  0 51959E+02 ppm1      4 557 ppm2      1 817
OR { 7742}
   (( segid "BrD " and resid 106  and name HA  ))
   (( segid "BrD " and resid 102  and name HB2 ))
ASSI { 8052}
   (( segid "BrD " and resid 77   and name HB1 ))
   (( segid "BrD " and resid 80   and name HB2 ))
     3 300     2 700     2 200 peak  8052 weight  0 10000E+01 volume  0 59988E+02 ppm1      3 325 ppm2      2 564
OR { 8052}
   (( segid "BrD " and resid 77   and name HB1 ))
   (( segid "BrD " and resid 54   and name HB1 ))
OR { 8052}
   (( segid "BrD " and resid 77   and name HB1 ))
   ( segid "BrD " and resid 54   and name HE% )
ASSI { 8122}
   (( segid "BrD " and resid 63   and name HA  ))
   (( segid "BrD " and resid 62   and name HB1 ))
     3 700     3 400     1 800 peak  8122 weight  0 10000E+01 volume  0.30661E+02 ppm1      5 296 ppm2      2 660
OR { 8122}
   (( segid "BrD " and resid 63   and name HA  ))
   (( segid "BrD " and resid 67   and name HB2 ))
OR { 8122}
   (( segid "BrD " and resid 63   and name HA  ))
   (( segid "BrD " and resid 64   and name HB1 ))
ASSI { 8212}
   (( segid "BrD " and resid 109  and name HG1 ))
   (( segid "BrD " and resid 109  and name HB1 ))
     2 200     1 200     1 200 peak  8212 weight  0 10000E+01 volume  0 72542E+03 ppm1      1 401 ppm2      2 310
OR { 8212}
   ( segid "BrD " and resid 14   and name HD2%)
   (( segid "BrD " and resid 18   and name HG  ))
ASSI { 8492}
   ( segid "BrD " and resid 18   and name HD2%)
   (( segid "BrD " and resid 14   and name HA  ))
     2 700     1 800     1 800 peak  8492 weight  0 10000E+01 volume  0 19700E+03 ppm1      0 414 ppm2      4 626
OR { 8492}
   ( segid "BrD " and resid 18   and name HD2%)
   (( segid "BrD " and resid 15   and name HA  ))
OR { 8492}
   ( segid "BrD " and resid 18   and name HD2%)
   (( segid "BrD " and resid 71   and name HA  ))
ASSI { 8542}
   ( segid "BrD " and resid 22   and name HD1%)
   (( segid "BrD " and resid 60   and name HB2 ))
     2 600     1 700     1.700 peak  8542 weight  0 10000E+01 volume  0 24926E+03 ppm1      1 645 ppm2      4 629
OR { 8542}
   ( segid "BrD " and resid 22   and name HD1%)
   (( segid "BrD " and resid 23   and name HA  ))
OR { 8542}
   ( segid "BrD " and resid 22   and name HD1%)
   (( segid "BrD " and resid 56   and name HA  ))
OR { 8542}
   ( segid "BrD " and resid 22   and name HD1%)
   (( segid "BrD " and resid 61   and name HA  ))
ASSI { 8662}
   ( segid "BrD " and resid 56   and name HD2%)
   ( segid "BrD " and resid 22   and name HD2%)
     2 200     1.200     1 200 peak  8662 weight  0 10000E+01 volume  0.65442E+03 ppm1      1 254 ppm2      1 635
OR { 8662}
   ( segid "BrD " and resid 56   and name HD2%)
   ( segid "BrD " and resid 25   and name HG2%)
ASSI { 8712}
   ( segid "BrD " and resid 56   and name HD1%)
   ( segid "BrD " and resid 102  and name HD1%)
     2.600     1.700     1 700 peak  8712 weight  0 10000E+01 volume  0.26563E+03 ppm1      1 547 ppm2      1 321
OR { 8712}
   ( segid "BrD " and resid 56   and name HD1%)
   ( segid "BrD " and resid 102  and name HD2%)
OR { 8712}
   (( segid "BrD " and resid 116  and name HG12))
   ( segid "BrD " and resid 115  and name HD1%)
ASSI { 8962}
   (( segid "BrD " and resid 56   and name HB2 ))
   ( segid "BrD " and resid 25   and name HG2%)
     3 700     3 400     1 800 peak  8962 weight  0 10000E+01 volume  0 31139E+02 ppm1      1 994 ppm2      1.627
OR { 8962}
   (( segid "BrD " and resid 102  and name HB1 ))
   ( segid "BrD " and resid 101  and name HG2%)
OR { 8962}
   (( segid "BrD " and resid 56   and name HB2 ))
   ( segid "BrD " and resid 22   and name HD2%)
ASSI { 9112}
   ( segid "BrD " and resid 21   and name HG2%)
   ( segid "BrD " and resid 102  and name HD2%)
     2 600     1 700     1 700 peak  9112 weight  0 10000E+01 volume  0 28598E+03 ppm1      1 600 ppm2      1 324
OR { 9112}
   ( segid "BrD " and resid 101  and name HG2%)
   ( segid "BrD " and resid 102  and name HD1%)
ASSI { 9142}
   ( segid "BrD " and resid 21   and name HG2%)
   ( segid "BrD " and resid 78   and name HD1%)
     3 800     3 600     1 700 peak  9142 weight  0 10000E+01 volume  0 27968E+02 ppm1      1 596 ppm2      0.772
OR { 9142}
   ( segid "BrD " and resid 21   and name HG2%)
   ( segid "BrD " and resid 81   and name HG2%)
ASSI { 9192}
   ( segid "BrD " and resid 21   and name HD1%)
   ( segid "BrD " and resid 18   and name HD1%)
     2 500     1 600     1.600 peak  9192 weight  0 10000E+01 volume  0 36076E+03 ppm1      1 205 ppm2      1 068
OR { 9192}
   ( segid "BrD " and resid 21   and name HD1%)
   (( segid "BrD " and resid 78   and name HB2 ))
ASSI { 9662}
   (( segid "BrD " and resid 79   and name HG1 ))
   ( segid "BrD " and resid 83   and name HG2%)
     3 000     2 200     2 200 peak  9662 weight  0 10000E+01 volume  0 10300E+03 ppm1      3.031 ppm2      1 900
OR { 9662}
   (( segid "BrD " and resid 79   and name HG1 ))
   (( segid "BrD " and resid 116  and name HG11))
ASSI {10002}
   (( segid "BrD " and resid 54   and name HB1 ))
   ( segid "BrD " and resid 81   and name HG1%)
     3.600     3.200     1 900 peak 10002 weight  0.10000E+01 volume  0.33897E+02 ppm1      2 585 ppm2      1 083
OR {10002}
   (( segid "BrD " and resid 42   and name HB2 ))
   ( segid "BrD " and resid 38   and name HG1%)
ASSI {10092}
   (( segid "BrD " and resid 35   and name HG1 ))
   (( segid "BrD " and resid 32   and name HA  ))
     3 100     2 400     2.400 peak 10092 weight  0 10000E+01 volume  0 97444E+02 ppm1      3 422 ppm2      4.972
OR {10092}
   (( segid "BrD " and resid 35   and name HG1 ))
   (( segid "BrD " and resid 31   and name HA  ))
ASSI {10182}
   (( segid "BrD " and resid 52   and name HB1 ))
   (( segid "BrD " and resid 80   and name HG1 ))
     4.100     4 100     1 400 peak 10182 weight  0 10000E+01 volume  0 17926E+02 ppm1      3 621 ppm2      2 345
OR {10182}
   (( segid "BrD " and resid 84   and name HB1 ))
   (( segid "BrD " and resid 80   and name HG1 ))
ASSI {10302}
   (( segid "BrD " and resid 42   and name HG1 ))
   (( segid "BrD " and resid 39   and name HD1 ))
     3.000     2.200     2.200 peak 10302 weight  0.10000E+01 volume  0 10808E+03 ppm1      2 880 ppm2      2 298
OR {10302}
   (( segid "BrD " and resid 7    and name HG1 ))
   (( segid "BrD " and resid 6    and name HB2 ))
ASSI {10412}
   (( segid "BrD " and resid 48   and name HA  ))
   (( segid "BrD " and resid 48   and name HB1 ))
     2 800     2.000     2 000 peak 10412 weight  0 10000E+01 volume  0 17461E+03 ppm1      4.831 ppm2      2.762
OR {10412}
   (( segid "BrD " and resid 87   and name HA  ))
   (( segid "BrD " and resid 87   and name HB1 ))
ASSI {10502}
   (( segid "BrD " and resid 112  and name HB1 ))
   ( segid "BrD " and resid 113  and name HB% )
     2 700     1 800     1.800 peak 10502 weight  0.10000E+01 volume  0 19681E+03 ppm1      2.684 ppm2      1 985
OR {10502}
   (( segid "BrD " and resid 112  and name HB1 ))
   (( segid "BrD " and resid 109  and name HD1 ))
ASSI {10602}
   (( segid "BrD " and resid 23   and name HA  ))
   (( segid "BrD " and resid 19   and name HA  ))
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    3 500      3 100      2.000 peak 10602 weight  0 10000E+01 volume  0 44566E+02 ppm1      4 656 ppm2      4 278
OR {10602}
  (( segid "BrD " and resid 104   and name HA  ))
  (( segid "BrD " and resid 101   and name HA  ))
ASSI {10902}
  (( segid "BrD " and resid 70    and name HB1 ))
  (( segid "BrD " and resid 11    and name HG1 ))
    3.200      2 600      2 300 peak 10902 weight  0 10000E+01 volume  0 71093E+02 ppm1      4 755 ppm2      2 646
OR {10902}
  (( segid "BrD " and resid 70    and name HB1 ))
  (  segid "BrD " and resid 75    and name HE% )
OR {10902}
  (( segid "BrD " and resid 93    and name HB2 ))
  (( segid "BrD " and resid 97    and name HB1 ))
OR {10902}
  (( segid "BrD " and resid 70    and name HB1 ))
  (( segid "BrD " and resid 62    and name HB1 ))
OR {10902}
  (( segid "BrD " and resid 70    and name HB1 ))
  (( segid "BrD " and resid 8     and name HG1 ))
ASSI {11592}
  (( segid "BrD " and resid 109   and name HB2 ))
  (  segid "BrD " and resid 21    and name HD1%)
    3 400      2.900      2 100 peak 11592 weight  0 10000E+01 volume  0 47549E+02 ppm1      2.141 ppm2      1 222
OR {11592}
  (( segid "BrD " and resid 109   and name HB2 ))
  (  segid "BrD " and resid 110   and name HG2%)
ASSI {11652}
  (( segid "BrD " and resid 59    and name HB2 ))
  (  segid "BrD " and resid 58    and name HG2%)
    2 900      2 100      2 100 peak 11652 weight  0 10000E+01 volume  0 12259E+03 ppm1      2.487 ppm2      1 660
OR {11652}
  (( segid "BrD " and resid 59    and name HB2 ))
  (  segid 'BrD " and resid 22    and name HD1%)
ASSI {12162}
  (( segid "BrD " and resid 18    and name HA  ))
  (  segid "BrD " and resid 21    and name HG2%)
    3 600      3 200      1.900 peak 12162 weight  0 10000E+01 volume  0 38701E+02 ppm1      3.866 ppm2      1 591
OR {12162}
  (( segid "BrD " and resid 18    and name HA  ))
  (  segid "BrD " and resid 22    and name HD2%)
ASSI {12172}
  (( segid "BrD " and resid 6     and name HA  ))
  (( segid "BrD " and resid 6     and name HG2 ))
    2 500      1 600      1.600 peak 12172 weight  0.10000E+01 volume  0 31535E+03 ppm1      4 951 ppm2      2 033
OR {12172}
  (( segid "BrD " and resid 39    and name HA  ))
  (( segid "BrD " and resid 39    and name HG1 ))
ASSI {12302}
  (( segid "BrD " and resid 86    and name HG2 ))
  (( segid "BrD " and resid 83    and name HA  ))
    3.600      3 200      1.900 peak 12302 weight  0 10000E+01 volume  0 36612E+02 ppm1      0.760 ppm2      4 450
OR {12302}
  (( segid "BrD " and resid 86    and name HG2 ))
  (( segid "BrD " and resid 96    and name HA  ))
ASSI {12572}
  (  segid "BrD " and resid 59    and name HE% )
  (  segid "BrD " and resid 22    and name HD1%)
    2 700      1.800      1 800 peak 12572 weight  0 10000E+01 volume  0 19213E+03 ppm1      1 848 ppm2      1 645
OR {12572}
  (  segid "BrD " and resid 59    and name HE% )
  (  segid "BrD " and resid 63    and name HD1%)
ASSI {12722}
  (  segid "BrD " and resid 18    and name HD1%)
  (( segid "BrD " and resid 68    and name HB2 ))
    3 400      2 900      2 100 peak 12722 weight  0 10000E+01 volume  0 56232E+02 ppm1      1.056 ppm2      3.513
OR {12722}
  (  segid "BrD " and resid 18    and name HD1%)
  (( segid "BrD " and resid 75    and name HG1 ))
ASSI {12742}
  (( segid "BrD " and resid 72    and name HA  ))
  (  segid "BrD " and resid 116   and name HG2%)
    3 000      2 200      2 200 peak 12742 weight  0 10000E+01 volume  0 10372E+03 ppm1      4.656 ppm2      1 414
OR {12742}
  (( segid "BrD " and resid 67    and name HA  ))
  (  segid "BrD " and resid 69    and name HG2%)
OR {12742}
  (( segid "BrD " and resid 111   and name HA  ))
  (  segid "BrD " and resid 116   and name HD1%)
ASSI {12862}
  (( segid "BrD " and resid 62    and name HD1 ))
  (  segid "BrD " and resid 54    and name HE% )
    3 000      2 200      2.200 peak 12862 weight  0.10000E+01 volume  0 10219E+03 ppm1      3 177 ppm2      2.569
OR {12862}
  (( segid "BrD " and resid 62    and name HD1 ))
  (( segid "BrD " and resid 63    and name HB2 ))
OR {12862}
  (( segid "BrD " and resid 62    and name HD1 ))
  (( segid "BrD " and resid 54    and name HB1 ))
ASSI {13242}
  (( segid "BrD " and resid 46    and name HB2 ))
  (  segid "BrD " and resid 38    and name HG2%)
    3 500      3 100      2 000 peak 13242 weight  0 10000E+01 volume  0 46826E+02 ppm1      3 080 ppm2      0 791
OR {13242}
  (( segid "BrD " and resid 46    and name HB2 ))
  (( segid "BrD " and resid 50    and name HG12))
ASSI {13322}
  (  segid "BrD " and resid 78    and name HD2%)
  (  segid "BrD " and resid 21    and name HG2%)
    2 700      1 800      1 800 peak 13322 weight  0.10000E+01 volume  0 21424E+03 ppm1      0 662 ppm2      1 590
OR {13322}
  (  segid "BrD " and resid 78    and name HD2%)
  (  segid "BrD " and resid 22    and name HD2%)
ASSI {13352}
  (  segid "BrD " and resid 18    and name HD2%)
  (( segid "BrD " and resid 14    and name HB1 ))
    4 200      4 200      1 300 peak 13352 weight  0.10000E+01 volume  0 14748E+02 ppm1      0.415 ppm2      2 481
OR {13352}
  (  segid "BrD " and resid 18    and name HD2%)
  (( segid "BrD " and resid 21    and name HB  ))
ASSI {13392}
  (  segid "BrD " and resid 25    and name HG1%)
  (( segid "BrD " and resid 28    and name HA  ))
    2 800      2 000      2 000 peak 13392 weight  0 10000E+01 volume  0.16152E+03 ppm1      1 795 ppm2      4 566
OR {13392}
  (  segid "BrD " and resid 25    and name HG1%)
  (( segid "BrD " and resid 106   and name HA  ))
ASSI {13592}
  (  segid "BrD " and resid 56    and name HD2%)
  (( segid "BrD " and resid 59    and name HB2 ))
    2 600      1 700      1 700 peak 13592 weight  0 10000E+01 volume  0 24679E+03 ppm1      1 254 ppm2      2 499
OR {13592}
  (  segid "BrD " and resid 56    and name HD2%)
  (  segid "BrD " and resid 54    and name HE% )
OR {13592}
  (  segid "BrD " and resid 56    and name HD2%)
  (( segid "BrD " and resid 26    and name HB1 ))
ASSI {13602}
  (  segid "BrD " and resid 54    and name HE% )
  (( segid "BrD " and resid 37    and name HB2 ))
    2 500      1 600      1 600 peak 13602 weight  0 10000E+01 volume  0 34655E+03 ppm1      2 535 ppm2      2 323
OR {13602}
  (  segid "BrD " and resid 54    and name HE% )
  (( segid "BrD " and resid 56    and name HG  ))
ASSI {13762}
  (  segid "BrD " and resid 63    and name HD2%)
  (( segid "BrD " and resid 19    and name HB1 ))
    2 300      1 300      1 300 peak 13762 weight  0 10000E+01 volume  0 59623E+03 ppm1      1 498 ppm2      2 318
OR {13762}
  (  segid "BrD " and resid 63    and name HD2%)
  (( segid "BrD " and resid 22    and name HB2 ))
ASSI {13952}
  (  segid "BrD " and resid 14    and name HD1%)
  (( segid "BrD " and resid 14    and name HA  ))
    2.700      1 800      1 800 peak 13952 weight  0 10000E+01 volume  0 20695E+03 ppm1      1 402 ppm2      4 687
OR {13952}
  (  segid "BrD " and resid 14    and name HD1%)
  (( segid "BrD " and resid 69    and name HA  ))
ASSI {14042}
  (  segid "BrD " and resid 76    and name HB% )
  (  segid "BrD " and resid 73    and name HD1%)
    3 100      2 400      2.400 peak 14042 weight  0.10000E+01 volume  0 97985E+02 ppm1      2 092 ppm2      1.540
OR {14042}
  (  segid "BrD " and resid 76    and name HB% )
  (( segid "BrD " and resid 116   and name HG12))
ASSI {14162}
  (( segid "BrD " and resid 15    and name HA  ))
  (  segid "BrD " and resid 63    and name HD2%)
    3 600      3.200      1 900 peak 14162 weight  0 10000E+01 volume  0 37938E+02 ppm1      4 609 ppm2      1 490
OR {14162}
  (( segid "BrD " and resid 60    and name HB2 ))
  (  segid "BrD " and resid 63    and name HD2%)
ASSI {14192}
  (( segid "BrD " and resid 62    and name HA  ))
  (( segid "BrD " and resid 68    and name HB2 ))
    3.700      3 400      1 800 peak 14192 weight  0.10000E+01 volume  0.29812E+02 ppm1      4 459 ppm2      3 504
OR {14192}
  (( segid "BrD " and resid 95    and name HA  ))
  (( segid "BrD " and resid 89    and name HB2 ))
ASSI {14202}
  (( segid "BrD " and resid 95    and name HA  ))
  (( segid "BrD " and resid 98    and name HB2 ))
    3.200      2 600      2.300 peak 14202 weight  0 10000E+01 volume  0 81269E+02 ppm1      4 462 ppm2      3 701
OR {14202}
  (( segid "BrD " and resid 62    and name HA  ))
  (( segid "BrD " and resid 68    and name HB1 ))
ASSI {14312}
  (  segid "BrD " and resid 22    and name HD2%)
  (( segid "BrD " and resid 59    and name HB2 ))
    2 700      1 800      1 800 peak 14312 weight  0.10000E+01 volume  0.21510E+03 ppm1      1 599 ppm2      2 501
OR {14312}
  (  segid "BrD " and resid 22    and name HD2%)
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  (( segid "BrD " and resid 21   and name HB  ))
OR {14312}
  (  segid "BrD " and resid 22   and name HD2%)
  (( segid "BrD " and resid 63   and name HB2 ))
OR {14312}
  (  segid "BrD " and resid 22   and name HD2%)
  (( segid "BrD " and resid 26   and name HB1 ))
ASSI {14432}
  (  segid "BrD " and resid 21   and name HD1%)
  (( segid "BrD " and resid 18   and name HB1 ))
    2 700     1 800     1.800 peak 14432 weight  0 10000E+01 volume  0 19246E+03 ppm1    1 205 ppm2    2 148
OR {14432}
  (  segid "BrD " and resid 21   and name HD1%)
  (( segid "BrD " and resid 102  and name HG  ))
ASSI {14462}
  (  segid "BrD " and resid 110  and name HD1%)
  (  segid "BrD " and resid 116  and name HD1%)
    2 100     1 100     1 100 peak 14462 weight  0.10000E+01 volume  0 89267E+03 ppm1    1 154 ppm2    1 387
OR {14462}
  (  segid "BrD " and resid 110  and name HD1%)
  (  segid "BrD " and resid 115  and name HD1%)
ASSI {14602}
  (  segid "BrD " and resid 18   and name HD1%)
  (  segid "BrD " and resid 115  and name HD1%)
    3 500     3 100     2.000 peak 14602 weight  0 10000E+01 volume  0 42578E+02 ppm1    1 057 ppm2    1 327
OR {14602}
  (  segid "BrD " and resid 18   and name HD1%)
  (( segid "BrD " and resid 78   and name HB1 ))
ASSI {14642}
  (( segid "BrD " and resid 18   and name HA  ))
  (  segid "BrD " and resid 102  and name HD2%)
    4 400     4 400     1 100 peak 14642 weight  0 10000E+01 volume  0.11486E+02 ppm1    3.867 ppm2    1 320
OR {14642}
  (( segid "BrD " and resid 18   and name HA  ))
  (  segid "BrD " and resid 115  and name HD1%)
OR {14642}
  (( segid "BrD " and resid 18   and name HA  ))
  (( segid "BrD " and resid 78   and name HB1 ))
ASSI {14682}
  (  segid "BrD " and resid 22   and name HD1%)
  (( segid "BrD " and resid 64   and name HG1 ))
    3 000     2 200     2 200 peak 14682 weight  0 10000E+01 volume  0 10496E+03 ppm1    1 645 ppm2    2 186
OR {14682}
  (( segid "BrD " and resid 110  and name HG12))
  (( segid "BrD " and resid 115  and name HB1 ))
ASSI {14692}
  (  segid "BrD " and resid 63   and name HD2%)
  (( segid "BrD " and resid 19   and name HD1 ))
    2 300     1 300     1 300 peak 14692 weight  0 10000E+01 volume  0 59246E+03 ppm1    1 498 ppm2    2 191
OR {14692}
  (  segid "BrD " and resid 63   and name HD2%)
  (( segid "BrD " and resid 64   and name HG1 ))
ASSI {14792}
  (  segid "BrD " and resid 22   and name HD2%)
  (( segid "BrD " and resid 56   and name HA  ))
    2.600     1 700     1 700 peak 14792 weight  0 10000E+01 volume  0 26795E+03 ppm1    1 599 ppm2    4 639
OR {14792}
  (  segid "BrD " and resid 22   and name HD2%)
  (( segid "BrD " and resid 60   and name HB2 ))
ASSI {14802}
  (( segid "BrD " and resid 86   and name HD1 ))
  (( segid "BrD " and resid 83   and name HA  ))
    2 700     1 800     1.800 peak 14802 weight  0 10000E+01 volume  0 19483E+03 ppm1    1 896 ppm2    4.461
OR {14802}
  (( segid "BrD " and resid 103  and name HB2 ))
  (( segid "BrD " and resid 99   and name HA  ))
ASSI {14862}
  (( segid "BrD " and resid 54   and name HA  ))
  (  segid "BrD " and resid 81   and name HG1%)
    3 800     3 600     1 700 peak 14862 weight  0.10000E+01 volume  0 25126E+02 ppm1    5 543 ppm2    1 076
OR {14862}
  (( segid "BrD " and resid 54   and name HA  ))
  (  segid "BrD " and resid 38   and name HG1%)
ASSI {14872}
  (  segid "BrD " and resid 81   and name HG1%)
  (( segid "BrD " and resid 80   and name HB2 ))
    2 900     2.100     2 100 peak 14872 weight  0 10000E+01 volume  0 14378E+03 ppm1    1.058 ppm2    2 565
OR {14872}
  (  segid "BrD " and resid 81   and name HG1%)
  (( segid "BrD " and resid 80   and name HB1 ))
OR {14872}
  (  segid "BrD " and resid 81   and name HG1%)
  (  segid "BrD " and resid 54   and name HE% )
OR {14872}
  (  segid "BrD " and resid 81   and name HG1%)
  (( segid "BrD " and resid 54   and name HB1 ))
ASSI {14882}
  (  segid "BrD " and resid 81   and name HG1%)
  (( segid "BrD " and resid 56   and name HG  ))
    3 500     3 100     2 000 peak 14882 weight  0 10000E+01 volume  0 44935E+02 ppm1    1.058 ppm2    2 328
OR {14882}
  (  segid "BrD " and resid 38   and name HG1%)
  (( segid "BrD " and resid 37   and name HB2 ))
ASSI {15202}
  (( segid "BrD " and resid 72   and name HA  ))
  (( segid "BrD " and resid 75   and name HG2 ))
    4 000     4 000     1.500 peak 15202 weight  0 10000E+01 volume  0 18586E+02 ppm1    4 656 ppm2    3.224
OR {15202}
  (( segid "BrD " and resid 61   and name HA  ))
  (( segid "BrD " and resid 59   and name HG2 ))
OR {15202}
  (( segid "BrD " and resid 61   and name HA  ))
  (( segid "BrD " and resid 59   and name HG1 ))
ASSI {15382}
  (( segid "BrD " and resid 74   and name HA  ))
  (  segid "BrD " and resid 75   and name HE% )
    3 200     2 600     2 300 peak 15382 weight  0 10000E+01 volume  0 70547E+02 ppm1    4 362 ppm2    2.653
OR {15382}
  (( segid "BrD " and resid 74   and name HA  ))
  (( segid "BrD " and resid 59   and name HB1 ))
ASSI {15392}
  (( segid "BrD " and resid 74   and name HB1 ))
  (( segid "BrD " and resid 73   and name HB2 ))
    3 200     2 600     2.300 peak 15392 weight  0 10000E+01 volume  0 74692E+02 ppm1    3.572 ppm2    2 471
OR {15392}
  (( segid "BrD " and resid 74   and name HB1 ))
  (( segid "BrD " and resid 63   and name HG  ))
ASSI {15532}
  (( segid "BrD " and resid 82   and name HB2 ))
  (( segid "BrD " and resid 103  and name HB1 ))
    3 100     2.400     2 400 peak 15532 weight  0 10000E+01 volume  0 91508E+02 ppm1    3.573 ppm2    2 344
OR {15532}
  (( segid "BrD " and resid 82   and name HB2 ))
  (( segid "BrD " and resid 86   and name HB1 ))
ASSI {15542}
  (( segid "BrD " and resid 82   and name HB1 ))
  (( segid "BrD " and resid 103  and name HB1 ))
    3 100     2 400     2 400 peak 15542 weight  0 10000E+01 volume  0 94295E+02 ppm1    3 672 ppm2    2 344
OR {15542}
  (( segid "BrD " and resid 107  and name HB1 ))
  (( segid "BrD " and resid 110  and name HB  ))
OR {15542}
  (( segid "BrD " and resid 107  and name HB1 ))
  (( segid "BrD " and resid 103  and name HB1 ))
OR {15542}
  (( segid "BrD " and resid 106  and name HB2 ))
  (( segid "BrD " and resid 109  and name HB1 ))
OR {15542}
  (( segid "BrD " and resid 106  and name HB2 ))
  (( segid "BrD " and resid 21   and name HG11))
ASSI {15562}
  (( segid "BrD " and resid 82   and name HB1 ))
  (( segid "BrD " and resid 103  and name HB2 ))
    3 500     3.100     2 000 peak 15562 weight  0 10000E+01 volume  0 43748E+02 ppm1    3 671 ppm2    1 897
OR {15562}
  (( segid "BrD " and resid 82   and name HB1 ))
  (  segid "BrD " and resid 83   and name HG2%)
ASSI {15572}
  (( segid "BrD " and resid 106  and name HB2 ))
  (( segid "BrD " and resid 110  and name HG11))
    5 500     5 500     0 000 peak 15572 weight  0 10000E+01 volume  0 17071E+01 ppm1    3.671 ppm2    1 722
OR {15572}
  (( segid "BrD " and resid 107  and name HB1 ))
  (( segid "BrD " and resid 110  and name HG11))
OR {15572}
  (( segid "BrD " and resid 106  and name HB2 ))
  (  segid "BrD " and resid 17   and name HG2%)
ASSI {15582}
  (( segid "BrD " and resid 15   and name HB2 ))
  (  segid "BrD " and resid 63   and name HD1%)
    3 300     2 700     2 200 peak 15582 weight  0 10000E+01 volume  0 63482E+02 ppm1    3 671 ppm2    1 653
OR {15582}
  (( segid "BrD " and resid 106  and name HB2 ))
  (( segid "BrD " and resid 110  and name HG12))
OR {15582}
  (( segid "BrD " and resid 107  and name HB1 ))
  (( segid "BrD " and resid 110  and name HG12))
ASSI {15722}
  (( segid "BrD " and resid 52   and name HB1 ))
  (( segid "BrD " and resid 80   and name HB1 ))
    4 700     4 700     0.800 peak 15722 weight  0.10000E+01 volume  0 74610E+01 ppm1    3 620 ppm2    2 597
OR {15722}
  (( segid "BrD " and resid 84   and name HB1 ))
  (( segid "BrD " and resid 87   and name HB2 ))
OR {15722}
  (( segid "BrD " and resid 84   and name HB1 ))
  (( segid "BrD " and resid 80   and name HB1 ))
OR {15722}
  (( segid "BrD " and resid 65   and name HB1 ))
  (( segid "BrD " and resid 64   and name HB1 ))
ASSI {16012}
  (( segid "BrD " and resid 68   and name HA  ))
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   ( segid "BrD " and resid 69   and name HG2%)
     3 700     3 400     1 800 peak 16012 weight  0 10000E+01 volume  0 30406E+02 ppm1      5 148 ppm2      1 433
OR {16012}
   (( segid "BrD " and resid 68   and name HA  ))
   ( segid "BrD " and resid 14   and name HD2%)
ASSI {16172}
   (( segid "BrD " and resid 68   and name HB1 ))
   ( segid "BrD " and resid 63   and name HD1%)
     3 600     3 200     1 900 peak 16172 weight  0 10000E+01 volume  0 37293E+02 ppm1      3 668 ppm2      1 645
OR {16172}
   (( segid "BrD " and resid 68   and name HB1 ))
   ( segid "BrD " and resid 22   and name HD1%)
ASSI {16182}
   (( segid "BrD " and resid 68   and name HB2 ))
   ( segid "BrD " and resid 63   and name HD1%)
     3 800     3 600     1 700 peak 16182 weight  0 10000E+01 volume  0 27740E+02 ppm1      3 522 ppm2      1 645
OR {16182}
   (( segid "BrD " and resid 68   and name HB2 ))
   ( segid "BrD " and resid 22   and name HD1%)
ASSI {16362}
   (( segid "BrD " and resid 97   and name HE1 ))
   ( segid "BrD " and resid 101  and name HD1%)
     3 000     2 200     2.200 peak 16362 weight  0 10000E+01 volume  0 11543E+03 ppm1      3 571 ppm2      1 580
OR {16362}
   (( segid "BrD " and resid 64   and name HE1 ))
   ( segid "BrD " and resid 22   and name HD2%)
OR {16362}
   (( segid "BrD " and resid 97   and name HE1 ))
   ( segid "BrD " and resid 101  and name HG2%)
ASSI {16372}
   (( segid "BrD " and resid 88   and name HB1 ))
   (( segid "BrD " and resid 50   and name HG11))
     2 900     2 100     2 100 peak 16372 weight  0 10000E+01 volume  0 13106E+03 ppm1      3 522 ppm2      1 401
OR {16372}
   (( segid "BrD " and resid 111  and name HE1 ))
   ( segid "BrD " and resid 116  and name HD1%)
ASSI {16482}
   (( segid "BrD " and resid 96   and name HA  ))
   (( segid "BrD " and resid 85   and name HB1 ))
     3 800     3 600     1 700 peak 16482 weight  0 10000E+01 volume  0 24633E+02 ppm1      4 409 ppm2      3 891
OR {16482}
   (( segid "BrD " and resid 107  and name HA  ))
   (( segid "BrD " and resid 106  and name HB1 ))
ASSI {16572}
   (( segid "BrD " and resid 96   and name HB2 ))
   (( segid "BrD " and resid 86   and name HA  ))
     4 100     4 100     1 400 peak 16572 weight  0 10000E+01 volume  0 16756E+02 ppm1      3.132 ppm2      4.804
OR {16572}
   (( segid "BrD " and resid 96   and name HB2 ))
   (( segid "BrD " and resid 92   and name HA  ))
ASSI {16582}
   (( segid "BrD " and resid 96   and name HB1 ))
   (( segid "BrD " and resid 92   and name HA  ))
     3 800     3 600     1 700 peak 16582 weight  0 10000E+01 volume  0 28094E+02 ppm1      4 004 ppm2      4 808
OR {16582}
   (( segid "BrD " and resid 96   and name HB1 ))
   (( segid "BrD " and resid 97   and name HA  ))
OR {16582}
   (( segid "BrD " and resid 96   and name HB1 ))
   (( segid "BrD " and resid 94   and name HA  ))
ASSI {16782}
   (( segid "BrD " and resid 95   and name HB1 ))
   (( segid "BrD " and resid 85   and name HA  ))
     3.200     2 600     2 300 peak 16782 weight  0 10000E+01 volume  0 73175E+02 ppm1      3 620 ppm2      4 995
OR {16782}
   (( segid "BrD " and resid 95   and name HB1 ))
   (( segid "BrD " and resid 93   and name HB1 ))
OR {16782}
   (( segid "BrD " and resid 84   and name HB1 ))
   (( segid "BrD " and resid 85   and name HA  ))
ASSI {16852}
   (( segid "BrD " and resid 82   and name HB1 ))
   ( segid "BrD " and resid 107  and name HE% )
     3 000     2 200     2 200 peak 16852 weight  0 10000E+01 volume  0.10680E+03 ppm1      3 670 ppm2      7 896
OR {16852}
   (( segid "BrD " and resid 107  and name HB1 ))
   ( segid "BrD " and resid 107  and name HE% )
ASSI {17112}
   (( segid "BrD " and resid 95   and name HB2 ))
   (( segid "BrD " and resid 32   and name HH2 ))
     3 500     3 100     2 000 peak 17112 weight  0 10000E+01 volume  0 46090E+02 ppm1      3 366 ppm2      7.754
OR {17112}
   (( segid "BrD " and resid 95   and name HB2 ))
   ( segid "BrD " and resid 34   and name HE% )
OR {17112}
   (( segid "BrD " and resid 95   and name HB2 ))
   ( segid "BrD " and resid 96   and name HD% )
ASSI {17122}
   (( segid "BrD " and resid 105  and name HB1 ))
   ( segid "BrD " and resid 25   and name HG1%)
     3 400     2 900     2.100 peak 17122 weight  0 10000E+01 volume  0 47791E+02 ppm1      3 721 ppm2      1 824
OR {17122}
   (( segid "BrD " and resid 105  and name HB1 ))
   (( segid "BrD " and resid 102  and name HB2 ))
ASSI {17132}
   (( segid "BrD " and resid 106  and name HB2 ))
   (( segid "BrD " and resid 102  and name HB2 ))
     3 500     3.100     2.000 peak 17132 weight  0 10000E+01 volume  0 42104E+02 ppm1      3 668 ppm2      1 824
OR {17132}
   (( segid "BrD " and resid 105  and name HB2 ))
   ( segid "BrD " and resid 25   and name HG1%)
OR {17132}
   (( segid "BrD " and resid 106  and name HB2 ))
   ( segid "BrD " and resid 25   and name HG1%)
ASSI {17142}
   (( segid "BrD " and resid 106  and name HB2 ))
   ( segid "BrD " and resid 21   and name HG2%)
     3 700     3 400     1.800 peak 17142 weight  0.10000E+01 volume  0 28702E+02 ppm1      3.668 ppm2      1 612
OR {17142}
   (( segid "BrD " and resid 105  and name HB2 ))
   ( segid "BrD " and resid 101  and name HG2%)
OR {17142}
   (( segid "BrD " and resid 105  and name HB2 ))
   ( segid "BrD " and resid 21   and name HG2%)
ASSI {17272}
   (( segid "BrD " and resid 116  and name HA  ))
   ( segid "BrD " and resid 110  and name HG2%)
     4.000     4 000     1 500 peak 17272 weight  0 10000E+01 volume  0 18200E+02 ppm1      4 804 ppm2      1 262
OR {17272}
   (( segid "BrD " and resid 57   and name HA  ))
   ( segid "BrD " and resid 56   and name HD2%)
ASSI {17322}
   (( segid "BrD " and resid 59   and name HA  ))
   (( segid "BrD " and resid 62   and name HG2 ))
     4 200     4 200     1 300 peak 17322 weight  0 10000E+01 volume  0 13830E+02 ppm1      4.903 ppm2      1 490
OR {17322}
   (( segid "BrD " and resid 20   and name HA  ))
   ( segid "BrD " and resid 63   and name HD2%)
ASSI {17492}
   (( segid "BrD " and resid 34   and name HA  ))
   (( segid "BrD " and resid 31   and name HA  ))
     3 300     2.700     2 200 peak 17492 weight  0 10000E+01 volume  0 57702E+02 ppm1      5.544 ppm2      4 989
OR {17492}
   (( segid "BrD " and resid 34   and name HA  ))
   (( segid "BrD " and resid 32   and name HA  ))
ASSI {17522}
   (( segid "BrD " and resid 34   and name HA  ))
   ( segid "BrD " and resid 54   and name HE% )
     4.000     4 000     1 500 peak 17522 weight  0.10000E+01 volume  0 19574E+02 ppm1      5 544 ppm2      2.564
OR {17522}
   (( segid "BrD " and resid 34   and name HA  ))
   (( segid "BrD " and resid 37   and name HG2 ))
ASSI {17682}
   (( segid "BrD " and resid 33   and name HG1 ))
   (( segid "BrD " and resid 32   and name HE3 ))
     4 900     4 900     0 600 peak 17682 weight  0 10000E+01 volume  0 54467E+01 ppm1      0 859 ppm2      7.926
OR {17682}
   (( segid "BrD " and resid 33   and name HG1 ))
   (( segid "BrD " and resid 34   and name HZ  ))
ASSI {17692}
   (( segid "BrD " and resid 33   and name HG1 ))
   (( segid "BrD " and resid 32   and name HZ3 ))
     4 000     4 000     1 500 peak 17692 weight  0.10000E+01 volume  0 18980E+02 ppm1      0 859 ppm2      7 803
OR {17692}
   (( segid "BrD " and resid 33   and name HG1 ))
   ( segid "BrD " and resid 34   and name HE% )
ASSI {17702}
   (( segid "BrD " and resid 33   and name HG1 ))
   (( segid "BrD " and resid 32   and name HH2 ))
     4 100     4.100     1 400 peak 17702 weight  0 10000E+01 volume  0 16294E+02 ppm1      0 859 ppm2      7 745
OR {17702}
   (( segid "BrD " and resid 33   and name HG1 ))
   ( segid "BrD " and resid 34   and name HE% )
ASSI {17892}
   (( segid "BrD " and resid 33   and name HD1 ))
   ( segid "BrD " and resid 34   and name HD% )
     3 400     2 900     2 100 peak 17892 weight  0 10000E+01 volume  0.51743E+02 ppm1      2.783 ppm2      7 720
OR {17892}
   (( segid "BrD " and resid 33   and name HD1 ))
   (( segid "BrD " and resid 32   and name HH2 ))
ASSI {17972}
   (( segid "BrD " and resid 33   and name HB2 ))
   (( segid "BrD " and resid 32   and name HZ3 ))
     3 500     3 100     2 000 peak 17972 weight  0 10000E+01 volume  0.44678E+02 ppm1      -0 176 ppm2      7 789
OR {17972}
   (( segid "BrD " and resid 33   and name HB2 ))
   ( segid "BrD " and resid 34   and name HE% )
ASSI {18022}
   (( segid "BrD " and resid 59   and name HG2 ))
   (( segid "BrD " and resid 60   and name HB2 ))
     3 200     2 600     2.300 peak 18022 weight  0 10000E+01 volume  0.69853E+02 ppm1      3 227 ppm2      4.664
OR {18022}
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   (( segid "BrD " and resid 75   and name HG2 ))
   (( segid "BrD " and resid 72   and name HA  ))
OR (18022)
   (( segid "BrD " and resid 59   and name HG1 ))
   (( segid "BrD " and resid 60   and name HB2 ))
OR (18022)
   (( segid "BrD " and resid 59   and name HG2 ))
   (( segid "BrD " and resid 58   and name HB  ))
OR (18022)
   (( segid "BrD " and resid 59   and name HG1 ))
   (( segid "BrD " and resid 58   and name HB  ))
ASSI (18032)
   (( segid "BrD " and resid 75   and name HG2 ))
   (( segid "BrD " and resid 74   and name HB1 ))
      3 400     2 900     2 100 peak 18032 weight  0 10000E+01 volume  0.48637E+02 ppm1      3 226 ppm2      3 597
OR (18032)
   (( segid "BrD " and resid 59   and name HG1 ))
   (( segid "BrD " and resid 74   and name HB1 ))
OR (18032)
   (( segid "BrD " and resid 59   and name HG2 ))
   (( segid "BrD " and resid 74   and name HB1 ))
OR (18032)
   (( segid "BrD " and resid 59   and name HG1 ))
   (( segid "BrD " and resid 67   and name HB1 ))
ASSI (18252)
   (  segid "BrD " and resid 35   and name HE% )
   (( segid "BrD " and resid 60   and name HB2 ))
      3 500     3 100     2 000 peak 18252 weight  0 10000E+01 volume  0 44998E+02 ppm1      2 782 ppm2      4 631
OR (18252)
   (  segid "BrD " and resid 35   and name HE% )
   (( segid "BrD " and resid 56   and name HA  ))
ASSI (18332)
   (  segid "BrD " and resid 35   and name HE% )
   (( segid "BrD " and resid 25   and name HB  ))
      3 700     3 400     1.800 peak 18332 weight  0 10000E+01 volume  0 33097E+02 ppm1      2 782 ppm2      3 003
OR (18332)
   (  segid "BrD " and resid 35   and name HE% )
   (( segid "BrD " and resid 55   and name HB1 ))
ASSI (18342)
   (  segid "BrD " and resid 35   and name HE% )
   (( segid "BrD " and resid 35   and name HB1 ))
      1 700     1 700     2 800 peak 18342 weight  0 10000E+01 volume  0 31606E+04 ppm1      2 781 ppm2      2 841
OR (18342)
   (  segid "BrD " and resid 35   and name HE% )
   (( segid "BrD " and resid 57   and name HB2 ))
ASSI (18392)
   (  segid "BrD " and resid 35   and name HE% )
   (( segid "BrD " and resid 57   and name HD1 ))
      2 500     1 600     1 600 peak 18392 weight  0 10000E+01 volume  0 33173E+03 ppm1      2 782 ppm2      2 361
OR (18392)
   (  segid "BrD " and resid 35   and name HE% )
   (( segid "BrD " and resid 56   and name HG  ))
ASSI (18402)
   (  segid "BrD " and resid 35   and name HE% )
   (  segid "BrD " and resid 31   and name HB% )
      2 300     1 300     1.300 peak 18402 weight  0 10000E+01 volume  0 54118E+03 ppm1      2 782 ppm2      2 312
OR (18402)
   (  segid "BrD " and resid 35   and name HE% )
   (( segid "BrD " and resid 57   and name HD2 ))
OR (18402)
   (  segid "BrD " and resid 35   and name HE% )
   (( segid "BrD " and resid 56   and name HG  ))
ASSI (18432)
   (  segid "BrD " and resid 35   and name HE% )
   (( segid "BrD " and resid 57   and name HG1 ))
      2 800     2 000     2 000 peak 18432 weight  0.10000E+01 volume  0.16595E+03 ppm1      2 780 ppm2      2 118
OR (18432)
   (  segid "BrD " and resid 35   and name HE% )
   (( segid "BrD " and resid 26   and name HD1 ))
ASSI (18522)
   (  segid "BrD " and resid 75   and name HE% )
   (( segid "BrD " and resid 71   and name HA  ))
      2 600     1 700     1 700 peak 18522 weight  0.10000E+01 volume  0 24378E+03 ppm1      2 635 ppm2      4 663
OR (18522)
   (  segid "BrD " and resid 75   and name HE% )
   (( segid "BrD " and resid 14   and name HA  ))
ASSI (18532)
   (  segid "BrD " and resid 75   and name HE% )
   (( segid "BrD " and resid 110  and name HA  ))
      4 200     4 200     1.300 peak 18532 weight  0.10000E+01 volume  0 13873E+02 ppm1      2.633 ppm2      4 383
OR (18532)
   (  segid "BrD " and resid 75   and name HE% )
   (( segid "BrD " and resid 74   and name HA  ))
ASSI (18592)
   (  segid "BrD " and resid 75   and name HE% )
   (  segid "BrD " and resid 74   and name HE% )
      3 600     3 200     1.900 peak 18592 weight  0 10000E+01 volume  0 36365E+02 ppm1      2 634 ppm2      7 552
OR (18592)
   (  segid "BrD " and resid 75   and name HE% )
   (  segid "BrD " and resid 106  and name HD% )
ASSI (18822)
   (  segid "BrD " and resid 75   and name HE% )
   (( segid "BrD " and resid 116  and name HG12))
      3 300     2.700     2 200 peak 18822 weight  0 10000E+01 volume  0 58075E+02 ppm1      2 635 ppm2      1 588
OR (18822)
   (  segid "BrD " and resid 75   and name HE% )
   (  segid "BrD " and resid 21   and name HG2%)
ASSI (18832)
   (  segid "BrD " and resid 75   and name HE% )
   (  segid "BrD " and resid 63   and name HD1%)
      3 400     2 900     2 100 peak 18832 weight  0.10000E+01 volume  0 54622E+02 ppm1      2.635 ppm2      1 657
OR (18832)
   (  segid "BrD " and resid 75   and name HE% )
   (( segid "BrD " and resid 110  and name HG12))
OR (18832)
   (  segid "BrD " and resid 75   and name HE% )
   (( segid "BrD " and resid 21   and name HG12))
ASSI (18912)
   (  segid "BrD " and resid 75   and name HE% )
   (( segid "BrD " and resid 14   and name HB2 ))
      2 700     1 800     1 800 peak 18912 weight  0 10000E+01 volume  0 20227E+03 ppm1      2 635 ppm2      2 126
OR (18912)
   (  segid "BrD " and resid 75   and name HE% )
   (( segid "BrD " and resid 115  and name HG  ))
ASSI (18942)
   (  segid "BrD " and resid 75   and name HE% )
   (( segid "BrD " and resid 21   and name HG11))
      3 700     3.400     1 800 peak 18942 weight  0 10000E+01 volume  0 30880E+02 ppm1      2 636 ppm2      2 344
OR (18942)
   (  segid "BrD " and resid 75   and name HE% )
   (( segid "BrD " and resid 110  and name HB  ))
OR (18942)
   (  segid "BrD " and resid 75   and name HE% )
   (( segid "BrD " and resid 109  and name HB1 ))
ASSI (18962)
   (( segid "BrD " and resid 57   and name HB1 ))
   (( segid "BrD " and resid 37   and name HD1 ))
      3 100     2.400     2 400 peak 18962 weight  0 10000E+01 volume  0 84483E+02 ppm1      2 931 ppm2      4 289
OR (18962)
   (( segid "BrD " and resid 37   and name HB1 ))
   (( segid "BrD " and resid 37   and name HD1 ))
ASSI (19022)
   (( segid "BrD " and resid 75   and name HA  ))
   (( segid "BrD " and resid 78   and name HB2 ))
      2.500     1 600     1 600 peak 19022 weight  0.10000E+01 volume  0 30551E+03 ppm1      4.508 ppm2      1 043
OR (19022)
   (( segid "BrD " and resid 75   and name HA  ))
   (  segid "BrD " and resid 18   and name HD1%)
ASSI (19222)
   (  segid "BrD " and resid 43   and name HB% )
   (( segid "BrD " and resid 42   and name HB1 ))
      4 500     4.500     1 000 peak 19222 weight  0 10000E+01 volume  0 92899E+01 ppm1      1.697 ppm2      2 768
OR (19222)
   (  segid "BrD " and resid 43   and name HB% )
   (( segid "BrD " and resid 44   and name HG1 ))
ASSI (19332)
   (  segid "BrD " and resid 31   and name HB% )
   (( segid "BrD " and resid 26   and name HB1 ))
      3.600     3 200     1 900 peak 19332 weight  0.10000E+01 volume  0 33671E+02 ppm1      2 289 ppm2      2 466
OR (19332)
   (  segid "BrD " and resid 31   and name HB% )
   (( segid "BrD " and resid 21   and name HB  ))
ASSI (19342)
   (  segid "BrD " and resid 31   and name HB% )
   (( segid "BrD " and resid 56   and name HB1 ))
      3.300     2 700     2 200 peak 19342 weight  0.10000E+01 volume  0 60076E+02 ppm1      2.289 ppm2      2 719
OR (19342)
   (  segid "BrD " and resid 31   and name HB% )
   (( segid "BrD " and resid 29   and name HB1 ))
ASSI (19402)
   (  segid "BrD " and resid 31   and name HB% )
   (( segid "BrD " and resid 29   and name HA  ))
      3 600     3 200     1 900 peak 19402 weight  0 10000E+01 volume  0 34186E+02 ppm1      2 289 ppm2      4 810
OR (19402)
   (  segid "BrD " and resid 31   and name HB% )
   (( segid "BrD " and resid 24   and name HA  ))
ASSI (19452)
   (( segid "BrD " and resid 73   and name HB2 ))
   (( segid "BrD " and resid 72   and name HA  ))
      3 800     3.600     1.700 peak 19452 weight  0.10000E+01 volume  0.27108E+02 ppm1      2.486 ppm2      4 672
OR (19452)
   (( segid "BrD " and resid 73   and name HB2 ))
   (( segid "BrD " and resid 69   and name HA  ))
ASSI (19462)
   (( segid "BrD " and resid 73   and name HB1 ))
   (( segid "BrD " and resid 72   and name HA  ))
      3.900     3.800     1 600 peak 19462 weight  0.10000E+01 volume  0.22158E+02 ppm1      2.583 ppm2      4 672
OR (19462)
   (( segid "BrD " and resid 73   and name HB1 ))
   (( segid "BrD " and resid 69   and name HA  ))
ASSI (19472)
   (  segid "BrD " and resid 99   and name HB% )
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  (( segid "BrD " and resid 86   and name HB1 ))
    2.400     1.400     1.400 peak 19472 weight  0 10000E+01 volume  0 42620E+03 ppm1      2.190 ppm2      2 359
OR {19472}
  (  segid "BrD " and resid 99   and name HB% )
  (( segid "BrD " and resid 103  and name HB1 ))
ASSI {19562}
  (  segid "BrD " and resid 76   and name HB% )
  (( segid "BrD " and resid 51   and name HB1 ))
    1 800     1 800     2 700 peak 19562 weight  0 10000E+01 volume  0 21948E+04 ppm1      2 092 ppm2      1 946
OR {19562}
  (  segid "BrD " and resid 76   and name HB% )
  (( segid "BrD " and resid 116  and name HG11))
OR {19562}
  (  segid "BrD " and resid 76   and name HB% )
  (( segid "BrD " and resid 51   and name HG1 ))
ASSI {19712}
  (  segid "BrD " and resid 99   and name HB% )
  (( segid "BrD " and resid 98   and name HB1 ))
    3 300     2 700     2.200 peak 19712 weight  0 10000E+01 volume  0 62693E+02 ppm1      2 190 ppm2      3 988
OR {19712}
  (  segid "BrD " and resid 99   and name HB% )
  (( segid "BrD " and resid 96   and name HB1 ))
ASSI {19862}
  (( segid "BrD " and resid 102  and name HA  ))
  (( segid "BrD " and resid 105  and name HA  ))
    4 200     4 200     1 300 peak 19862 weight  0 10000E+01 volume  0.13941E+02 ppm1      4 261 ppm2      4 924
OR {19862}
  (( segid "BrD " and resid 102  and name HA  ))
  (( segid "BrD " and resid 30   and name HB1 ))
ASSI {19872}
  (( segid "BrD " and resid 102  and name HA  ))
  (  segid "BrD " and resid 105  and name HD% )
    2 700     1 800     1 800 peak 19872 weight  0 10000E+01 volume  0 22737E+03 ppm1      4 261 ppm2      7 779
OR {19872}
  (( segid "BrD " and resid 102  and name HA  ))
  (  segid "BrD " and resid 34   and name HE% )
ASSI {19892}
  (( segid "BrD " and resid 113  and name HA  ))
  (( segid "BrD " and resid 115  and name HG  ))
    3 600     3 200     1 900 peak 19892 weight  0 10000E+01 volume  0.36454E+02 ppm1      4 903 ppm2      2 133
OR {19892}
  (( segid "BrD " and resid 113  and name HA  ))
  (( segid "BrD " and resid 14   and name HB2 ))
ASSI {19932}
  (( segid "BrD " and resid 113  and name HA  ))
  (( segid "BrD " and resid 112  and name HA  ))
    3 400     2 900     2 100 peak 19932 weight  0 10000E+01 volume  0 55030E+02 ppm1      4 903 ppm2      4 598
OR {19932}
  (( segid "BrD " and resid 113  and name HA  ))
  (( segid "BrD " and resid 114  and name HA1 ))
ASSI {19972}
  (  segid "BrD " and resid 113  and name HB% )
  (  segid "BrD " and resid 75   and name HE% )
    3 400     2 900     2 100 peak 19972 weight  0.10000E+01 volume  0 53194E+02 ppm1      1.991 ppm2      2 662
OR {19972}
  (  segid "BrD " and resid 113  and name HB% )
  (( segid "BrD " and resid 112  and name HB1 ))
ASSI {20002}
  (  segid "BrD " and resid 113  and name HB% )
  (( segid "BrD " and resid 18   and name HG  ))
    2 700     1 800     1 800 peak 20002 weight  0 10000E+01 volume  0 18667E+03 ppm1      1 991 ppm2      2 304
OR {20002}
  (  segid "BrD " and resid 113  and name HB% )
  (( segid "BrD " and resid 110  and name HB  ))
OR {20002}
  (  segid "BrD " and resid 113  and name HB% )
  (( segid "BrD " and resid 109  and name HB1 ))
ASSI {20012}
  (  segid "BrD " and resid 113  and name HB% )
  (( segid "BrD " and resid 110  and name HB  ))
    3 900     3 800     1 600 peak 20012 weight  0 10000E+01 volume  0.22660E+02 ppm1      1.990 ppm2      2.369
OR {20012}
  (  segid "BrD " and resid 113  and name HB% )
  (( segid "BrD " and resid 109  and name HB1 ))
ASSI {20022}
  (  segid "BrD " and resid 113  and name HB% )
  (( segid "BrD " and resid 115  and name HG  ))
    3 300     2 700     2.200 peak 20022 weight  0 10000E+01 volume  0 61319E+02 ppm1      1 990 ppm2      2 135
OR {20022}
  (  segid "BrD " and resid 113  and name HB% )
  (( segid "BrD " and resid 14   and name HB2 ))
ASSI {20062}
  (( segid "BrD " and resid 110  and name HA  ))
  (  segid "BrD " and resid 116  and name HD1%)
    3.100     2 400     2 400 peak 20062 weight  0 10000E+01 volume  0.82911E+02 ppm1      4.411 ppm2      1.410
OR {20062}
  (( segid "BrD " and resid 110  and name HA  ))
  (( segid "BrD " and resid 109  and name HG1 ))
ASSI {20122}
  (  segid "BrD " and resid 113  and name HB% )
  (( segid "BrD " and resid 114  and name HA1 ))
    3.700     3 400     1 800 peak 20122 weight  0 10000E+01 volume  0.29578E+02 ppm1      1 994 ppm2      4.564
OR {20122}
  (  segid "BrD " and resid 113  and name HB% )
  (( segid "BrD " and resid 17   and name HA  ))
ASSI {20152}
  (  segid "BrD " and resid 113  and name HB% )
  (  segid "BrD " and resid 14   and name HD1%)
    2 700     1 800     1 800 peak 20152 weight  0 10000E+01 volume  0.21357E+03 ppm1      1.995 ppm2      1 425
OR {20152}
  (  segid "BrD " and resid 113  and name HB% )
  (  segid "BrD " and resid 14   and name HD2%)
OR {20152}
  (  segid "BrD " and resid 113  and name HB% )
  (( segid "BrD " and resid 109  and name HG1 ))
ASSI {20182}
  (( segid "BrD " and resid 17   and name HB  ))
  (( segid "BrD " and resid 14   and name HB2 ))
    3 400     2 900     2 100 peak 20182 weight  0 10000E+01 volume  0 54504E+02 ppm1      4 853 ppm2      2 149
OR {20182}
  (( segid "BrD " and resid 17   and name HB  ))
  (( segid "BrD " and resid 18   and name HB1 ))
OR {20182}
  (( segid "BrD " and resid 17   and name HB  ))
  (( segid "BrD " and resid 109  and name HB2 ))
ASSI {20202}
  (( segid "BrD " and resid 17   and name HB  ))
  (  segid "BrD " and resid 21   and name HD1%)
    4 300     4 300     1 200 peak 20202 weight  0 10000E+01 volume  0 12632E+02 ppm1      4 853 ppm2      1 222
OR {20202}
  (( segid "BrD " and resid 17   and name HB  ))
  (  segid "BrD " and resid 110  and name HG2%)
ASSI {20222}
  (  segid "BrD " and resid 17   and name HG2%)
  (( segid "BrD " and resid 14   and name HA  ))
    2 200     1 200     1 200 peak 20222 weight  0 10000E+01 volume  0 69704E+03 ppm1      1 747 ppm2      4 666
OR {20222}
  (  segid "BrD " and resid 17   and name HG2%)
  (( segid "BrD " and resid 109  and name HA  ))
OR {20222}
  (  segid "BrD " and resid 17   and name HG2%)
  (( segid "BrD " and resid 20   and name HB1 ))
ASSI {20262}
  (  segid "BrD " and resid 17   and name HG2%)
  (( segid "BrD " and resid 109  and name HB1 ))
    2 500     1 600     1 600 peak 20262 weight  0 10000E+01 volume  0 34655E+03 ppm1      1 747 ppm2      2 352
OR {20262}
  (  segid "BrD " and resid 17   and name HG2%)
  (( segid "BrD " and resid 21   and name HG11))
ASSI {20322}
  (( segid "BrD " and resid 20   and name HB1 ))
  (( segid "BrD " and resid 21   and name HG11))
    2 300     2.300     2 200 peak 20322 weight  0 10000E+01 volume  0 47335E+03 ppm1      4 656 ppm2      2 320
OR {20322}
  (( segid "BrD " and resid 20   and name HB1 ))
  (( segid "BrD " and resid 19   and name HB1 ))
OR {20322}
  (( segid "BrD " and resid 20   and name HB1 ))
  (( segid "BrD " and resid 109  and name HB1 ))
ASSI {20632}
  (( segid "BrD " and resid 112  and name HG2 ))
  (( segid "BrD " and resid 109  and name HD1 ))
    3 100     2 400     2 400 peak 20632 weight  0 10000E+01 volume  0 87177E+02 ppm1      2.832 ppm2      1 997
OR {20632}
  (( segid "BrD " and resid 112  and name HG2 ))
  (( segid "BrD " and resid 111  and name HG1 ))
OR {20632}
  (( segid "BrD " and resid 112  and name HG2 ))
  (  segid "BrD " and resid 113  and name HB% )
ASSI {20652}
  (( segid "BrD " and resid 111  and name HA  ))
  (  segid "BrD " and resid 115  and name HD1%)
    3.800     3 600     1 700 peak 20652 weight  0 10000E+01 volume  0 25940E+02 ppm1      4 656 ppm2      1 319
OR {20652}
  (( segid "BrD " and resid 104  and name HA  ))
  (  segid "BrD " and resid 102  and name HD2%)
OR {20652}
  (( segid "BrD " and resid 72   and name HA  ))
  (  segid "BrD " and resid 115  and name HD1%)
OR {20652}
  (( segid "BrD " and resid 104  and name HA  ))
  (  segid "BrD " and resid 102  and name HD1%)
OR {20652}
  (( segid "BrD " and resid 72   and name HA  ))
  (( segid "BrD " and resid 78   and name HB1 ))
ASSI {20662}
  (( segid "BrD " and resid 61   and name HA  ))
  (( segid "BrD " and resid 62   and name HB2 ))
    3 300     2 700     2 200 peak 20662 weight  0 10000E+01 volume  0 56653E+02 ppm1      4 656 ppm2      1 710
OR {20662}
  (( segid "BrD " and resid 67   and name HA  ))
  (( segid "BrD " and resid 62   and name HB2 ))
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OR {20662}
  (( segid "BrD " and resid 111  and name HA  ))
  (( segid "BrD " and resid 110  and name HG11))
ASSI {20672}
  (( segid "BrD " and resid 23   and name HA  ))
  (( segid "BrD " and resid 26   and name HG1 ))
    3 300     2 700     2 200 peak 20672 weight  0 10000E+01 volume  0 58313E+02 ppm1      4 656 ppm2      1 661
OR {20672}
  (( segid "BrD " and resid 23   and name HA  ))
  (  segid "BrD " and resid 22   and name HD1%)
OR {20672}
  (( segid "BrD " and resid 61   and name HA  ))
  (  segid "BrD " and resid 22   and name HD1%)
OR {20672}
  (( segid "BrD " and resid 61   and name HA  ))
  (( segid "BrD " and resid 62   and name HB2 ))
OR {20672}
  (( segid "BrD " and resid 23   and name HA  ))
  (  segid "BrD " and resid 25   and name HG2%)
OR {20672}
  (( segid "BrD " and resid 61   and name HA  ))
  (  segid "BrD " and resid 58   and name HG2%)
OR {20672}
  (( segid "BrD " and resid 67   and name HA  ))
  (( segid "BrD " and resid 62   and name HB2 ))
ASSI {20682}
  (( segid "BrD " and resid 67   and name HA  ))
  (  segid "BrD " and resid 69   and name HG1%)
    2 700     1 800     1 800 peak 20682 weight  0 10000E+01 volume  0 18983E+03 ppm1      4 656 ppm2      1 547
OR {20682}
  (( segid "BrD " and resid 67   and name HA  ))
  (  segid "BrD " and resid 73   and name HD1%)
ASSI {20792}
  (  segid "BrD " and resid 25   and name HG2%)
  (  segid "BrD " and resid 74   and name HE% )
    3 100     2 400     2 400 peak 20792 weight  0 10000E+01 volume  0 98567E+02 ppm1      1 648 ppm2      7 517
OR {20792}
  (  segid "BrD " and resid 25   and name HG2%)
  (  segid "BrD " and resid 106  and name HD% )
OR {20792}
  (  segid "BrD " and resid 58   and name HG2%)
  (  segid "BrD " and resid 74   and name HE% )
ASSI {20822}
  (  segid "BrD " and resid 25   and name HG2%)
  (  segid "BrD " and resid 34   and name HE% )
    3.300     2 700     2.200 peak 20822 weight  0 10000E+01 volume  0 60371E+02 ppm1      1 650 ppm2      7 791
OR {20822}
  (  segid "BrD " and resid 58   and name HG2%)
  (  segid "BrD " and resid 68   and name HD% )
ASSI {20842}
  (  segid "BrD " and resid 25   and name HG2%)
  (( segid "BrD " and resid 102  and name HA  ))
    3 600     3 200     1.900 peak 20842 weight  0 10000E+01 volume  0 35063E+02 ppm1      1 649 ppm2      4 282
OR {20842}
  (  segid "BrD " and resid 58   and name HG2%)
  (( segid "BrD " and resid 37   and name HD1 ))
ASSI {21092}
  (  segid "BrD " and resid 58   and name HG2%)
  (( segid "BrD " and resid 61   and name HG2 ))
    2 600     1 700     1 700 peak 21092 weight  0 10000E+01 volume  0 23144E+03 ppm1      1 648 ppm2      2 833
OR {21092}
  (  segid "BrD " and resid 58   and name HG2%)
  (( segid "BrD " and resid 61   and name HB1 ))
OR {21092}
  (  segid "BrD " and resid 58   and name HG2%)
  (( segid "BrD " and resid 57   and name HB2 ))
ASSI {21102}
  (  segid "BrD " and resid 25   and name HG2%)
  (( segid "BrD " and resid 56   and name HB1 ))
    2 500     1 600     1.600 peak 21102 weight  0 10000E+01 volume  0 34384E+03 ppm1      1 649 ppm2      2 700
OR {21102}
  (  segid "BrD " and resid 58   and name HG2%)
  (( segid "BrD " and resid 61   and name HB2 ))
OR {21102}
  (  segid "BrD " and resid 58   and name HG2%)
  (( segid "BrD " and resid 37   and name HG1 ))
OR {21102}
  (  segid "BrD " and resid 25   and name HG2%)
  (( segid "BrD " and resid 22   and name HB1 ))
ASSI {21112}
  (  segid "BrD " and resid 58   and name HG2%)
  (  segid "BrD " and resid 54   and name HE% )
    2 500     1 600     1 600 peak 21112 weight  0 10000E+01 volume  0 32059E+03 ppm1      1 649 ppm2      2.508
OR {21112}
  (  segid "BrD " and resid 25   and name HG2%)
  (( segid "BrD " and resid 26   and name HB1 ))
ASSI {21132}
  (( segid "BrD " and resid 83   and name HB  ))
  (( segid "BrD " and resid 79   and name HG1 ))
    5 000     5 000     0 500 peak 21132 weight  0 10000E+01 volume  0.54051E+01 ppm1      4 804 ppm2      3 028
OR {21132}
  (( segid "BrD " and resid 83   and name HB  ))
  (( segid "BrD " and resid 87   and name HG1 ))
ASSI {21152}
  (( segid "BrD " and resid 58   and name HA  ))
  (  segid "BrD " and resid 54   and name HE% )
    3.500     3.100     2 000 peak 21152 weight  0 10000E+01 volume  0 43944E+02 ppm1      4 459 ppm2      2 572
OR {21152}
  (( segid "BrD " and resid 83   and name HA  ))
  (( segid "BrD " and resid 87   and name HB2 ))
ASSI {21222}
  (  segid "BrD " and resid 83   and name HG2%)
  (( segid "BrD " and resid 80   and name HG1 ))
    3 000     2 200     2.200 peak 21222 weight  0 10000E+01 volume  0 98918E+02 ppm1      1 894 ppm2      2.366
OR {21222}
  (  segid "BrD " and resid 83   and name HG2%)
  (( segid "BrD " and resid 86   and name HB1 ))
ASSI {21382}
  (( segid "BrD " and resid 25   and name HB  ))
  (  segid "BrD " and resid 102  and name HD1%)
    5 400     5 400     0 100 peak 21382 weight  0 10000E+01 volume  0 33579E+01 ppm1      2 980 ppm2      1 273
OR {21382}
  (( segid "BrD " and resid 25   and name HB  ))
  (  segid "BrD " and resid 56   and name HD2%)
ASSI {21432}
  (  segid "BrD " and resid 25   and name HG1%)
  (  segid "BrD " and resid 31   and name HB% )
    3 300     2 700     2.200 peak 21432 weight  0 10000E+01 volume  0 60830E+02 ppm1      1 795 ppm2      2 320
OR {21432}
  (  segid "BrD " and resid 25   and name HG1%)
  (( segid "BrD " and resid 21   and name HG11))
ASSI {21442}
  (  segid "BrD " and resid 25   and name HG1%)
  (( segid "BrD " and resid 105  and name HB1 ))
    2 600     1 700     1 700 peak 21442 weight  0 10000E+01 volume  0 23532E+03 ppm1      1 796 ppm2      3.695
OR {21442}
  (  segid "BrD " and resid 25   and name HG1%)
  (( segid "BrD " and resid 105  and name HB2 ))
OR {21442}
  (  segid "BrD " and resid 25   and name HG1%)
  (( segid "BrD " and resid 106  and name HB2 ))
ASSI {21502}
  (( segid "BrD " and resid 38   and name HA  ))
  (( segid "BrD " and resid 39   and name HD1 ))
    3 600     3 200     1.900 peak 21502 weight  0 10000E+01 volume  0.37412E+02 ppm1      4 163 ppm2      2 291
OR {21502}
  (( segid "BrD " and resid 38   and name HA  ))
  (( segid "BrD " and resid 37   and name HB2 ))
ASSI {21552}
  (  segid "BrD " and resid 81   and name HG2%)
  (( segid "BrD " and resid 31   and name HA  ))
    3 000     2.200     2 200 peak 21552 weight  0 10000E+01 volume  0 11144E+03 ppm1      0 760 ppm2      4 981
OR {21552}
  (  segid "BrD " and resid 81   and name HG2%)
  (( segid "BrD " and resid 85   and name HA  ))
OR {21552}
  (  segid "BrD " and resid 81   and name HG2%)
  (( segid "BrD " and resid 77   and name HA  ))
ASSI {21572}
  (  segid "BrD " and resid 81   and name HG1%)
  (( segid "BrD " and resid 77   and name HA  ))
    3 200     2 600     2.300 peak 21572 weight  0 10000E+01 volume  0 78059E+02 ppm1      1 056 ppm2      4 972
OR {21572}
  (  segid "BrD " and resid 38   and name HG1%)
  (( segid "BrD " and resid 39   and name HA  ))
ASSI {21592}
  (  segid "BrD " and resid 38   and name HG1%)
  (( segid "BrD " and resid 53   and name HA  ))
    3 100     2 400     2 400 peak 21592 weight  0 10000E+01 volume  0.93082E+02 ppm1      1 056 ppm2      4 664
OR {21592}
  (  segid "BrD " and resid 81   and name HG1%)
  (( segid "BrD " and resid 80   and name HA  ))
OR {21592}
  (  segid "BrD " and resid 81   and name HG1%)
  (( segid "BrD " and resid 53   and name HA  ))
ASSI {21612}
  (  segid "BrD " and resid 38   and name HG1%)
  (( segid "BrD " and resid 37   and name HB1 ))
    3 800     3.600     1 700 peak 21612 weight  0 10000E+01 volume  0.25206E+02 ppm1      1.056 ppm2      2.966
OR {21612}
  (  segid "BrD " and resid 81   and name HG1%)
  (( segid "BrD " and resid 55   and name HB1 ))
ASSI {21652}
  (  segid "BrD " and resid 38   and name HG1%)
  (  segid "BrD " and resid 47   and name HE% )
    3 100     2 400     2 400 peak 21652 weight  0 10000E+01 volume  0 89355E+02 ppm1      1 056 ppm2      7 259
OR {21652}
  (  segid "BrD " and resid 81   and name HG1%)
  (  segid "BrD " and resid 82   and name HD% )
ASSI {21792}
  (( segid "BrD " and resid 81   and name HB  ))
  (( segid "BrD " and resid 82   and name HB2 ))
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   3.900     3.800     1.600 peak 21792 weight  0 10000E+01 volume  0 21639E+02 ppm1      2.042 ppm2      3.573
OR {21792}
  (( segid "BrD " and resid 81   and name HB  ))
  (( segid "BrD " and resid 84   and name HB1 ))
ASSI {21982}
  (  segid "BrD " and resid 50   and name HD1%)
  (( segid "BrD " and resid 49   and name HA  ))
   3 000     2 200     2 200 peak 21982 weight  0.10000E+01 volume  0 11219E+03 ppm1      1 153 ppm2      4 692
OR {21982}
  (  segid "BrD " and resid 50   and name HD1%)
  (( segid "BrD " and resid 53   and name HA  ))
OR {21982}
  (  segid "BrD " and resid 50   and name HD1%)
  (( segid "BrD " and resid 47   and name HA  ))
ASSI {22072}
  (  segid "BrD " and resid 50   and name HD1%)
  (  segid "BrD " and resid 38   and name HG1%)
   3.800     3 600     1 700 peak 22072 weight  0 10000E+01 volume  0 25153E+02 ppm1      1 154 ppm2      1.078
OR {22072}
  (  segid "BrD " and resid 50   and name HD1%)
  (  segid "BrD " and resid 81   and name HG1%)
ASSI {22432}
  (  segid "BrD " and resid 69   and name HG2%)
  (( segid "BrD " and resid 19   and name HB2 ))
   5 500     5 500     0 000 peak 22432 weight  0.10000E+01 volume  0 51248E+00 ppm1      1 425 ppm2      1 993
OR {22432}
  (  segid "BrD " and resid 69   and name HG2%)
  (  segid "BrD " and resid 113  and name HB% )
ASSI {22502}
  (  segid "BrD " and resid 25   and name HG2%)
  (  segid "BrD " and resid 35   and name HE% )
   2.900     2 100     2 100 peak 22502 weight  0 10000E+01 volume  0 14480E+03 ppm1      1 633 ppm2      2 752
OR {22502}
  (  segid "BrD " and resid 49   and name HG1%)
  (( segid "BrD " and resid 48   and name HB1 ))
OR {22502}
  (  segid "BrD " and resid 58   and name HG2%)
  (( segid "BrD " and resid 37   and name HG1 ))
ASSI {22622}
  (( segid "BrD " and resid 42   and name HA  ))
  (( segid "BrD " and resid 44   and name HD2 ))
   4 000     4 000     1 500 peak 22622 weight  0.10000E+01 volume  0 20863E+02 ppm1      5 051 ppm2      4 133
OR {22622}
  (( segid "BrD " and resid 42   and name HA  ))
  (( segid "BrD " and resid 38   and name HA  ))
ASSI {22802}
  (( segid "BrD " and resid 104  and name HB1 ))
  (( segid "BrD " and resid 105  and name HB2 ))
   3 200     2 600     2 300 peak 22802 weight  0 10000E+01 volume  0 76681E+02 ppm1      2 536 ppm2      3 662
OR {22802}
  (( segid "BrD " and resid 104  and name HB1 ))
  (( segid "BrD " and resid 107  and name HB1 ))
ASSI {22862}
  (( segid "BrD " and resid 64   and name HE1 ))
  (( segid "BrD " and resid 19   and name HA  ))
   3.600     3 200     1.900 peak 22862 weight  0 10000E+01 volume  0 38596E+02 ppm1      3 573 ppm2      4 285
OR {22862}
  (( segid "BrD " and resid 57   and name HE1 ))
  (( segid "BrD " and resid 37   and name HD1 ))
ASSI {22912}
  (( segid "BrD " and resid 60   and name HB1 ))
  (( segid "BrD " and resid 22   and name HB2 ))
   4 100     4 100     1 400 peak 22912 weight  0 10000E+01 volume  0.16339E+02 ppm1      5.001 ppm2      2.312
OR {22912}
  (( segid "BrD " and resid 60   and name HB1 ))
  (( segid "BrD " and resid 56   and name HG  ))
ASSI {23002}
  (( segid "BrD " and resid 37   and name HD1 ))
  (( segid "BrD " and resid 57   and name HB1 ))
   3 100     2.400     2 400 peak 23002 weight  0 10000E+01 volume  0.82823E+02 ppm1      4 285 ppm2      2 966
OR {23002}
  (( segid "BrD " and resid 37   and name HD1 ))
  (( segid "BrD " and resid 37   and name HB1 ))
OR {23002}
  (( segid "BrD " and resid 44   and name HD1 ))
  (( segid "BrD " and resid 44   and name HB1 ))
ASSI {23042}
  (( segid "BrD " and resid 37   and name HD1 ))
  (( segid "BrD " and resid 37   and name HG2 ))
   2 000     1.000     1 000 peak 23042 weight  0 10000E+01 volume  0 14416E+04 ppm1      4.261 ppm2      2 621
OR {23042}
  (( segid "BrD " and resid 8    and name HD2 ))
  (( segid "BrD " and resid 8    and name HG1 ))
ASSI {23052}
  (( segid "BrD " and resid 8    and name HD1 ))
  (( segid "BrD " and resid 8    and name HB2 ))
   3 600     3.200     1 900 peak 23052 weight  0 10000E+01 volume  0.37937E+02 ppm1      4 409 ppm2      2.499
OR {23052}
  (( segid "BrD " and resid 8    and name HD1 ))
  (( segid "BrD " and resid 7    and name HB2 ))
ASSI {23212}
  (( segid "BrD " and resid 44   and name HG2 ))
  (( segid "BrD " and resid 44   and name HA  ))
   3.100     2 400     2 400 peak 23212 weight  0.10000E+01 volume  0 93859E+02 ppm1      2 635 ppm2      5 120
OR {23212}
  (( segid "BrD " and resid 8    and name HG1 ))
  (( segid "BrD " and resid 7    and name HA  ))
ASSI {23252}
  (( segid "BrD " and resid 11   and name HG1 ))
  (  segid "BrD " and resid 69   and name HG2%)
   3 000     2 200     2 200 peak 23252 weight  0 10000E+01 volume  0.10852E+03 ppm1      2 635 ppm2      1 417
OR {23252}
  (( segid "BrD " and resid 11   and name HG1 ))
  (  segid "BrD " and resid 14   and name HD2%)
ASSI {23382}
  (( segid "BrD " and resid 100  and name HA  ))
  (( segid "BrD " and resid 101  and name HA  ))
   5 500     5 500     0.000 peak 23382 weight  0 10000E+01 volume  0 24494E+01 ppm1      4 952 ppm2      4 256
OR {23382}
  (( segid "BrD " and resid 6    and name HA  ))
  (( segid "BrD " and resid 8    and name HD2 ))
ASSI {23392}
  (( segid "BrD " and resid 100  and name HA  ))
  (( segid "BrD " and resid 99   and name HA  ))
   3 200     2 600     2 300 peak 23392 weight  0 10000E+01 volume  0 72079E+02 ppm1      4 952 ppm2      4 444
OR {23392}
  (( segid "BrD " and resid 6    and name HA  ))
  (( segid "BrD " and resid 8    and name HD1 ))
ASSI {23512}
  (( segid "BrD " and resid 10   and name HA  ))
  (( segid "BrD " and resid 11   and name HA  ))
   3 400     2 900     2 100 peak 23512 weight  0 10000E+01 volume  0 53886E+02 ppm1      5 477 ppm2      4 939
OR {23512}
  (( segid "BrD " and resid 10   and name HA  ))
  (( segid "BrD " and resid 9    and name HA  ))
ASSI {23582}
  (( segid "BrD " and resid 12   and name HA  ))
  (( segid "BrD " and resid 15   and name HA  ))
   3 600     3 200     1 900 peak 23582 weight  0 10000E+01 volume  0 33831E+02 ppm1      5 297 ppm2      4 627
OR {23582}
  (( segid "BrD " and resid 12   and name HA  ))
  (( segid "BrD " and resid 16   and name HB1 ))
OR {23582}
  (( segid "BrD " and resid 12   and name HA  ))
  (( segid "BrD " and resid 14   and name HA  ))
ASSI {23682}
  (( segid "BrD " and resid 14   and name HA  ))
  (  segid "BrD " and resid 18   and name HD1%)
   3 300     2 700     2.200 peak 23682 weight  0.10000E+01 volume  0 67221E+02 ppm1      4 656 ppm2      1 083
OR {23682}
  (( segid "BrD " and resid 80   and name HA  ))
  (  segid "BrD " and resid 81   and name HG1%)
ASSI {23772}
  (  segid "BrD " and resid 14   and name HD2%)
  (( segid "BrD " and resid 15   and name HA  ))
   2 400     1 400     1 400 peak 23772 weight  0.10000E+01 volume  0 36871E+03 ppm1      1.400 ppm2      4 574
OR {23772}
  (( segid "BrD " and resid 109  and name HG1 ))
  (( segid "BrD " and resid 17   and name HA  ))
ASSI {23792}
  (  segid "BrD " and resid 14   and name HD2%)
  (( segid "BrD " and resid 18   and name HA  ))
   3 900     3 800     1.600 peak 23792 weight  0 10000E+01 volume  0 23831E+02 ppm1      1 401 ppm2      3 889
OR {23792}
  (( segid "BrD " and resid 109  and name HG1 ))
  (( segid "BrD " and resid 18   and name HA  ))
ASSI {23872}
  (( segid "BrD " and resid 18   and name HA  ))
  (  segid "BrD " and resid 74   and name HE% )
   2 900     2 100     2.100 peak 23872 weight  0.10000E+01 volume  0.13092E+03 ppm1      3 866 ppm2      7 534
OR {23872}
  (( segid "BrD " and resid 18   and name HA  ))
  (  segid "BrD " and resid 106  and name HD% )
ASSI {23892}
  (( segid "BrD " and resid 18   and name HA  ))
  (( segid "BrD " and resid 15   and name HA  ))
   2 900     2 100     2 100 peak 23892 weight  0.10000E+01 volume  0 13327E+03 ppm1      3 867 ppm2      4 631
OR {23892}
  (( segid "BrD " and resid 18   and name HA  ))
  (( segid "BrD " and resid 20   and name HB1 ))
OR {23892}
  (( segid "BrD " and resid 18   and name HA  ))
  (( segid "BrD " and resid 14   and name HA  ))
ASSI {23902}
  (( segid "BrD " and resid 18   and name HA  ))
  (( segid "BrD " and resid 17   and name HA  ))
   3.800     3.600     1 700 peak 23902 weight  0.10000E+01 volume  0 26018E+02 ppm1      3 867 ppm2      4 541
OR {23902}
  (( segid "BrD " and resid 18   and name HA  ))
  (( segid "BrD " and resid 106  and name HA  ))
ASSI {23912}
  (( segid "BrD " and resid 18   and name HB1 ))
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   ( segid "BrD " and resid 14   and name HD2%)
     3 400     2.900     2 100 peak 23912 weight  0 10000E+01 volume  0 53948E+02 ppm1     2 140 ppm2     1.433
OR {23912}
   (( segid "BrD " and resid 18   and name HB1 ))
   ( segid "BrD " and resid 69   and name HG2%)
ASSI {23942}
   (( segid "BrD " and resid 18   and name HB2 ))
   ( segid "BrD " and resid 14   and name HD2%)
     4 100     4.100     1 400 peak 23942 weight  0 10000E+01 volume  0 16641E+02 ppm1     0 911 ppm2     1 415
OR {23942}
   (( segid "BrD " and resid 18   and name HB2 ))
   ( segid "BrD " and resid 69   and name HG2%)
ASSI {24102}
   ( segid "BrD " and resid 18   and name HD2%)
   ( segid "BrD " and resid 21   and name HG2%)
     5 500     5 500     0 000 peak 24102 weight  0 10000E+01 volume  0 18200E+00 ppm1     0.415 ppm2     1 596
OR {24102}
   ( segid "BrD " and resid 18   and name HD2%)
   ( segid "BrD " and resid 22   and name HD2%)
ASSI {24112}
   ( segid "BrD " and resid 18   and name HD2%)
   ( segid "BrD " and resid 115  and name HD1%)
     2 800     2 000     2 000 peak 24112 weight  0 10000E+01 volume  0.15952E+03 ppm1     0 416 ppm2     1 377
OR {24112}
   ( segid "BrD " and resid 18   and name HD2%)
   ( segid "BrD " and resid 14   and name HD2%)
OR {24112}
   ( segid "BrD " and resid 18   and name HD2%)
   ( segid "BrD " and resid 14   and name HD1%)
ASSI {24122}
   ( segid "BrD " and resid 18   and name HD2%)
   ( segid "BrD " and resid 113  and name HB% )
     3 900     3 800     1 600 peak 24122 weight  0 10000E+01 volume  0 21517E+02 ppm1     0 415 ppm2     1 986
OR {24122}
   ( segid "BrD " and resid 18   and name HD2%)
   (( segid "BrD " and resid 19   and name HB2 ))
ASSI {24292}
   ( segid "BrD " and resid 18   and name HD2%)
   (( segid "BrD " and resid 106  and name HB2 ))
     3 900     3 800     1 600 peak 24292 weight  0 10000E+01 volume  0 23222E+02 ppm1     0 416 ppm2     3.650
OR {24292}
   ( segid "BrD " and resid 18   and name HD2%)
   (( segid "BrD " and resid 68   and name HB1 ))
OR {24292}
   ( segid "BrD " and resid 18   and name HD2%)
   (( segid "BrD " and resid 15   and name HB2 ))
ASSI {24492}
   ( segid "BrD " and resid 63   and name HD1%)
   (( segid "BrD " and resid 68   and name HB1 ))
     2 800     2 000     2 000 peak 24492 weight  0 10000E+01 volume  0 15293E+03 ppm1     1.649 ppm2     3.671
OR {24492}
   ( segid "BrD " and resid 63   and name HD1%)
   (( segid "BrD " and resid 15   and name HB2 ))
ASSI {24502}
   ( segid "BrD " and resid 63   and name HD1%)
   (( segid "BrD " and resid 66   and name HD2 ))
     3 000     2.200     2 200 peak 24502 weight  0 10000E+01 volume  0 10614E+03 ppm1     1 649 ppm2     3.614
OR {24502}
   ( segid "BrD " and resid 63   and name HD1%)
   (( segid "BrD " and resid 64   and name HE1 ))
ASSI {24532}
   ( segid "BrD " and resid 63   and name HD1%)
   (( segid "BrD " and resid 16   and name HA  ))
     3 500     3 100     2 000 peak 24532 weight  0 10000E+01 volume  0 45951E+02 ppm1     1 649 ppm2     4 516
OR {24532}
   ( segid "BrD " and resid 63   and name HD1%)
   (( segid "BrD " and resid 17   and name HA  ))
ASSI {24602}
   ( segid "BrD " and resid 63   and name HD2%)
   (( segid "BrD " and resid 19   and name HE1 ))
     3.400     2 900     2 100 peak 24602 weight  0 10000E+01 volume  0.54742E+02 ppm1     1 500 ppm2     3 524
OR {24602}
   ( segid "BrD " and resid 63   and name HD2%)
   (( segid "BrD " and resid 68   and name HB2 ))
ASSI {24692}
   (( segid "BrD " and resid 19   and name HA  ))
   (( segid "BrD " and resid 22   and name HG  ))
     3 000     2 200     2 200 peak 24692 weight  0.10000E+01 volume  0 10572E+03 ppm1     4.310 ppm2     2 393
OR {24692}
   (( segid "BrD " and resid 19   and name HA  ))
   (( segid "BrD " and resid 64   and name HD1 ))
ASSI {24712}
   (( segid "BrD " and resid 19   and name HA  ))
   (( segid "BrD " and resid 23   and name HA  ))
     3 700     3 400     1.800 peak 24712 weight  0 10000E+01 volume  0.31255E+02 ppm1     4 310 ppm2     4 677
OR {24712}
   (( segid "BrD " and resid 19   and name HA  ))
   (( segid "BrD " and resid 22   and name HA  ))
OR {24712}
   (( segid "BrD " and resid 19   and name HA  ))
   (( segid "BrD " and resid 20   and name HB1 ))
ASSI {24722}
   (( segid "BrD " and resid 19   and name HB2 ))
   (( segid "BrD " and resid 15   and name HA  ))
     3.800     3.600     1 700 peak 24722 weight  0 10000E+01 volume  0.24706E+02 ppm1     1 989 ppm2     4 576
OR {24722}
   (( segid "BrD " and resid 19   and name HB2 ))
   (( segid "BrD " and resid 16   and name HB1 ))
ASSI {24732}
   (( segid "BrD " and resid 19   and name HB2 ))
   (( segid "BrD " and resid 15   and name HA  ))
     3 800     3.600     1.700 peak 24732 weight  0 10000E+01 volume  0.28161E+02 ppm1     1.989 ppm2     4 631
OR {24732}
   (( segid "BrD " and resid 19   and name HB2 ))
   (( segid "BrD " and resid 20   and name HB1 ))
ASSI {24772}
   (( segid "BrD " and resid 19   and name HG1 ))
   (( segid "BrD " and resid 20   and name HA  ))
     4 200     4 200     1 300 peak 24772 weight  0 10000E+01 volume  0.15236E+02 ppm1     1 895 ppm2     4 891
OR {24772}
   (( segid "BrD " and resid 86   and name HG1 ))
   (( segid "BrD " and resid 87   and name HA  ))
OR {24772}
   (( segid "BrD " and resid 19   and name HG1 ))
   (( segid "BrD " and resid 64   and name HA  ))
ASSI {24822}
   (( segid "BrD " and resid 19   and name HD1 ))
   (( segid "BrD " and resid 15   and name HA  ))
     4.100     4 100     1 400 peak 24822 weight  0 10000E+01 volume  0 16533E+02 ppm1     2 190 ppm2     4 643
OR {24822}
   (( segid "BrD " and resid 19   and name HD1 ))
   (( segid "BrD " and resid 20   and name HB1 ))
ASSI {24852}
   (( segid "BrD " and resid 97   and name HE1 ))
   (( segid "BrD " and resid 97   and name HA  ))
     2.000     2 000     2 500 peak 24852 weight  0 10000E+01 volume  0.10950E+04 ppm1     3 571 ppm2     4 802
OR {24852}
   (( segid "BrD " and resid 57   and name HE1 ))
   (( segid "BrD " and resid 57   and name HA  ))
ASSI {24982}
   (( segid "BrD " and resid 21   and name HA  ))
   ( segid "BrD " and resid 106  and name HD% )
     3 600     3 200     1 900 peak 24982 weight  0 10000E+01 volume  0 38794E+02 ppm1     4 358 ppm2     7 517
OR {24982}
   (( segid "BrD " and resid 33   and name HA  ))
   ( segid "BrD " and resid 95   and name HD% )
ASSI {24992}
   (( segid "BrD " and resid 21   and name HA  ))
   (( segid "BrD " and resid 22   and name HA  ))
     2 000     2.000     2 500 peak 24992 weight  0 10000E+01 volume  0 12806E+04 ppm1     4 360 ppm2     4 671
OR {24992}
   (( segid "BrD " and resid 21   and name HA  ))
   (( segid "BrD " and resid 20   and name HB1 ))
ASSI {25052}
   (( segid "BrD " and resid 21   and name HG12))
   (( segid "BrD " and resid 18   and name HB1 ))
     3 500     3 100     2 000 peak 25052 weight  0 10000E+01 volume  0.40558E+02 ppm1     1 648 ppm2     2.141
OR {25052}
   (( segid "BrD " and resid 21   and name HG12))
   (( segid "BrD " and resid 109  and name HB2 ))
ASSI {25112}
   (( segid "BrD " and resid 21   and name HG12))
   (( segid "BrD " and resid 109  and name HG1 ))
     3.900     3 800     1 600 peak 25112 weight  0.10000E+01 volume  0 24225E+02 ppm1     1 648 ppm2     1 387
OR {25112}
   (( segid "BrD " and resid 21   and name HG12))
   ( segid "BrD " and resid 115  and name HD1%)
OR {25112}
   (( segid "BrD " and resid 21   and name HG12))
   ( segid "BrD " and resid 14   and name HD2%)
ASSI {25152}
   ( segid "BrD " and resid 21   and name HD1%)
   (( segid "BrD " and resid 106  and name HA  ))
     2 600     1 700     1 700 peak 25152 weight  0 10000E+01 volume  0 24691E+03 ppm1     1 205 ppm2     4.545
OR {25152}
   ( segid "BrD " and resid 21   and name HD1%)
   (( segid "BrD " and resid 17   and name HA  ))
OR {25152}
   ( segid "BrD " and resid 21   and name HD1%)
   (( segid "BrD " and resid 75   and name HA  ))
ASSI {25162}
   ( segid "BrD " and resid 21   and name HD1%)
   (( segid "BrD " and resid 20   and name HA  ))
     5 500     5 500     0 000 peak 25162 weight  0.10000E+01 volume  0 64481E-01 ppm1     1 205 ppm2     4 907
OR {25162}
   ( segid "BrD " and resid 21   and name HD1%)
   (( segid "BrD " and resid 105  and name HA  ))
OR {25162}
   ( segid "BrD " and resid 21   and name HD1%)
   (( segid "BrD " and resid 59   and name HA  ))
ASSI {25172}
   ( segid "BrD " and resid 21   and name HD1%)
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  (( segid "BrD " and resid 17   and name HB  ))
     3 100      2 400      2 400 peak 25172 weight  0 10000E+01 volume  0 95979E+02 ppm1      1.205 ppm2      4 863
OR {25172}
   (  segid "BrD " and resid 21   and name HD1%)
   (( segid "BrD " and resid 20   and name HA  ))
ASSI {25182}
   (  segid "BrD " and resid 21   and name HD1%)
   (  segid "BrD " and resid 74   and name HE% )
     2 600      1 700      1 700 peak 25182 weight  0 10000E+01 volume  0.25847E+03 ppm1      1 204 ppm2      7 536
OR {25182}
   (  segid "BrD " and resid 21   and name HD1%)
   (  segid "BrD " and resid 106  and name HD% )
ASSI {25392}
   (( segid "BrD " and resid 98   and name HA  ))
   (( segid "BrD " and resid 101  and name HA  ))
     3 400      2 900      2 100 peak 25392 weight  0 10000E+01 volume  0 50125E+02 ppm1      4 804 ppm2      4 265
OR {25392}
   (( segid "BrD " and resid 98   and name HA  ))
   (( segid "BrD " and resid 102  and name HA  ))
ASSI {25602}
   (  segid "BrD " and resid 21   and name HG2%)
   (( segid "BrD " and resid 20   and name HB1 ))
     3 400      2 900      2 100 peak 25602 weight  0 10000E+01 volume  0 54447E+02 ppm1      1 596 ppm2      4.657
OR {25602}
   (  segid "BrD " and resid 21   and name HG2%)
   (( segid "BrD " and resid 109  and name HA  ))
ASSI {25622}
   (  segid "BrD " and resid 21   and name HG2%)
   (( segid "BrD " and resid 105  and name HB1 ))
     3 400      2 900      2 100 peak 25622 weight  0 10000E+01 volume  0 55968E+02 ppm1      1 599 ppm2      3 736
OR {25622}
   (  segid "BrD " and resid 101  and name HG2%)
   (( segid "BrD " and resid 105  and name HB1 ))
ASSI {25632}
   (  segid "BrD " and resid 21   and name HG2%)
   (( segid "BrD " and resid 106  and name HB2 ))
     4 400      4 400      1 100 peak 25632 weight  0 10000E+01 volume  0 10843E+02 ppm1      1 599 ppm2      3 662
OR {25632}
   (  segid "BrD " and resid 21   and name HG2%)
   (( segid "BrD " and resid 105  and name HB2 ))
ASSI {25672}
   (  segid "BrD " and resid 101  and name HD1%)
   (( segid "BrD " and resid 97   and name HB1 ))
     3 100      2 400      2 400 peak 25672 weight  0 10000E+01 volume  0 84040E+02 ppm1      1.550 ppm2      2 702
OR {25672}
   (  segid "BrD " and resid 101  and name HD1%)
   (( segid "BrD " and resid 29   and name HB1 ))
ASSI {25692}
   (  segid "BrD " and resid 101  and name HD1%)
   (( segid "BrD " and resid 97   and name HG2 ))
     3 800      3 600      1 700 peak 25692 weight  0 10000E+01 volume  0 27614E+02 ppm1      1 550 ppm2      2 167
OR {25692}
   (  segid "BrD " and resid 101  and name HD1%)
   (  segid "BrD " and resid 99   and name HB% )
OR {25692}
   (  segid "BrD " and resid 101  and name HD1%)
   (( segid "BrD " and resid 33   and name HD2 ))
ASSI {25702}
   (  segid "BrD " and resid 21   and name HG2%)
   (  segid "BrD " and resid 75   and name HE% )
     4 300      4 300      1 200 peak 25702 weight  0 10000E+01 volume  0 11881E+02 ppm1      1 599 ppm2      2 654
OR {25702}
   (  segid "BrD " and resid 21   and name HG2%)
   (( segid "BrD " and resid 22   and name HB1 ))
OR {25702}
   (  segid "BrD " and resid 101  and name HG2%)
   (( segid "BrD " and resid 97   and name HB1 ))
ASSI {25732}
   (  segid "BrD " and resid 101  and name HG2%)
   (( segid "BrD " and resid 102  and name HB1 ))
     2 600      1.700      1 700 peak 25732 weight  0 10000E+01 volume  0 25581E+03 ppm1      1 599 ppm2      2 011
OR {25732}
   (  segid "BrD " and resid 21   and name HG2%)
   (( segid "BrD " and resid 109  and name HD1 ))
ASSI {25772}
   (  segid "BrD " and resid 21   and name HG2%)
   (  segid "BrD " and resid 18   and name HD1%)
     3.200      2.600      2 300 peak 25772 weight  0.10000E+01 volume  0 75349E+02 ppm1      1 599 ppm2      1 059
OR {25772}
   (  segid "BrD " and resid 21   and name HG2%)
   (( segid "BrD " and resid 78   and name HB2 ))
OR {25772}
   (  segid "BrD " and resid 21   and name HG2%)
   (  segid "BrD " and resid 81   and name HG1%)
ASSI {25832}
   (( segid "BrD " and resid 110  and name HB  ))
   (( segid "BrD " and resid 108  and name HA  ))
     3 800      3.600      1 700 peak 25832 weight  0 10000E+01 volume  0 26102E+02 ppm1      2.338 ppm2      4 823
OR {25832}
   (( segid "BrD " and resid 110  and name HB  ))
   (( segid "BrD " and resid 115  and name HA  ))
ASSI {25862}
   (  segid "BrD " and resid 110  and name HG2%)
   (( segid "BrD " and resid 114  and name HA2 ))
     3 100      2 400      2 400 peak 25862 weight  0 10000E+01 volume  0 90131E+02 ppm1      1 254 ppm2      4 509
OR {25862}
   (  segid "BrD " and resid 110  and name HG2%)
   (( segid "BrD " and resid 75   and name HA  ))
ASSI {25872}
   (  segid "BrD " and resid 110  and name HD1%)
   (( segid "BrD " and resid 14   and name HA  ))
     2 800      2 000      2 000 peak 25872 weight  0 10000E+01 volume  0 15256E+03 ppm1      1 154 ppm2      4 655
OR {25872}
   (  segid "BrD " and resid 110  and name HD1%)
   (( segid "BrD " and resid 71   and name HA  ))
OR {25872}
   (  segid "BrD " and resid 110  and name HD1%)
   (( segid "BrD " and resid 111  and name HA  ))
OR {25872}
   (  segid "BrD " and resid 110  and name HD1%)
   (( segid "BrD " and resid 109  and name HA  ))
ASSI {25882}
   (  segid "BrD " and resid 110  and name HG2%)
   (( segid "BrD " and resid 115  and name HA  ))
     2 800      2 000      2 000 peak 25882 weight  0 10000E+01 volume  0 15787E+03 ppm1      1 253 ppm2      4 824
OR {25882}
   (  segid "BrD " and resid 110  and name HG2%)
   (( segid "BrD " and resid 116  and name HA  ))
ASSI {25892}
   (  segid "BrD " and resid 110  and name HD1%)
   (( segid "BrD " and resid 17   and name HB  ))
     3 100      2 400      2 400 peak 25892 weight  0 10000E+01 volume  0 95882E+02 ppm1      1 154 ppm2      4.824
OR {25892}
   (  segid "BrD " and resid 110  and name HD1%)
   (( segid "BrD " and resid 115  and name HA  ))
ASSI {25902}
   (  segid "BrD " and resid 110  and name HD1%)
   (( segid "BrD " and resid 106  and name HA  ))
     3 000      2 200      2 200 peak 25902 weight  0 10000E+01 volume  0 11502E+03 ppm1      1 154 ppm2      4 568
OR {25902}
   (  segid "BrD " and resid 110  and name HD1%)
   (( segid "BrD " and resid 17   and name HA  ))
OR {25902}
   (  segid "BrD " and resid 110  and name HD1%)
   (( segid "BrD " and resid 114  and name HA1 ))
ASSI {26022}
   (  segid "BrD " and resid 110  and name HD1%)
   (( segid "BrD " and resid 106  and name HB2 ))
     3 200      2 600      2.300 peak 26022 weight  0 10000E+01 volume  0 70430E+02 ppm1      1 154 ppm2      3 670
OR {26022}
   (  segid "BrD " and resid 110  and name HD1%)
   (( segid "BrD " and resid 107  and name HB1 ))
ASSI {26042}
   (  segid "BrD " and resid 110  and name HG2%)
   (( segid "BrD " and resid 107  and name HB1 ))
     3 600      3 200      1 900 peak 26042 weight  0 10000E+01 volume  0 38059E+02 ppm1      1 251 ppm2      3.671
OR {26042}
   (  segid "BrD " and resid 110  and name HG2%)
   (( segid "BrD " and resid 106  and name HB2 ))
ASSI {26202}
   (  segid "BrD " and resid 116  and name HG2%)
   (( segid "BrD " and resid 76   and name HA  ))
     2.600      1.700      1 700 peak 26202 weight  0.10000E+01 volume  0 28885E+03 ppm1      1.401 ppm2      4 655
OR {26202}
   (  segid "BrD " and resid 116  and name HG2%)
   (( segid "BrD " and resid 72   and name HA  ))
ASSI {26312}
   (  segid "BrD " and resid 116  and name HD1%)
   (( segid "BrD " and resid 76   and name HA  ))
     3 800      3 600      1 700 peak 26312 weight  0 10000E+01 volume  0 26059E+02 ppm1      1 401 ppm2      4 655
OR {26312}
   (  segid "BrD " and resid 116  and name HD1%)
   (( segid "BrD " and resid 118  and name HA  ))
OR {26312}
   (  segid "BrD " and resid 116  and name HD1%)
   (( segid "BrD " and resid 111  and name HA  ))
OR {26312}
   (  segid "BrD " and resid 116  and name HD1%)
   (( segid "BrD " and resid 71   and name HA  ))
OR {26312}
   (  segid "BrD " and resid 116  and name HD1%)
   (( segid "BrD " and resid 72   and name HA  ))
ASSI {26352}
   (  segid "BrD " and resid 116  and name HG2%)
   (( segid "BrD " and resid 79   and name HA  ))
     3 600      3 200      1.900 peak 26352 weight  0 10000E+01 volume  0 36722E+02 ppm1      1 400 ppm2      4 428
OR {26352}
   (  segid "BrD " and resid 116  and name HG2%)
   (( segid "BrD " and resid 107  and name HA  ))
ASSI {26362}
   (  segid "BrD " and resid 116  and name HD1%)
   (( segid "BrD " and resid 107  and name HB1 ))
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    3 800     3 600     1 700 peak 26362 weight  0.10000E+01 volume  0 28562E+02 ppm1      1 401 ppm2      3 662
OR {26362}
  (  segid "BrD " and resid 116  and name HD1%)
  (( segid "BrD " and resid 106  and name HB2 ))
ASSI {26512}
  (( segid "BrD " and resid 116  and name HB  ))
  (( segid "BrD " and resid 76   and name HA  ))
    3.300     2.700     2 200 peak 26512 weight  0 10000E+01 volume  0 66907E+02 ppm1      2 410 ppm2      4 655
OR {26512}
  (( segid "BrD " and resid 116  and name HB  ))
  (( segid "BrD " and resid 118  and name HA  ))
OR {26512}
  (( segid "BrD " and resid 116  and name HB  ))
  (( segid "BrD " and resid 72   and name HA  ))
ASSI {27012}
  (( segid "BrD " and resid 89   and name HA  ))
  (( segid "BrD " and resid 88   and name HA  ))
    3.600     3.200     1 900 peak 27012 weight  0 10000E+01 volume  0 33743E+02 ppm1      5.642 ppm2      5.005
OR {27012}
  (( segid "BrD " and resid 89   and name HA  ))
  (( segid "BrD " and resid 93   and name HB1 ))
ASSI {27292}
  (( segid "BrD " and resid 80   and name HG1 ))
  (( segid "BrD " and resid 52   and name HB1 ))
    3 300     2 700     2.200 peak 27292 weight  0 10000E+01 volume  0 61197E+02 ppm1      2 341 ppm2      3 649
OR {27292}
  (( segid "BrD " and resid 73   and name HG  ))
  (( segid "BrD " and resid 68   and name HB1 ))
ASSI {27302}
  (( segid "BrD " and resid 80   and name HG1 ))
  (( segid "BrD " and resid 77   and name HB1 ))
    4 600     4 600     0 900 peak 27302 weight  0 10000E+01 volume  0 87654E+01 ppm1      2 341 ppm2      3 311
OR {27302}
  (( segid "BrD " and resid 73   and name HG  ))
  (( segid "BrD " and resid 77   and name HB1 ))
OR {27302}
  (( segid "BrD " and resid 73   and name HG  ))
  (( segid "BrD " and resid 54   and name HG1 ))
OR {27302}
  (( segid "BrD " and resid 56   and name HG  ))
  (( segid "BrD " and resid 54   and name HG1 ))
OR {27302}
  (( segid "BrD " and resid 56   and name HG  ))
  (( segid "BrD " and resid 77   and name HB1 ))
ASSI {27332}
  (( segid "BrD " and resid 56   and name HG  ))
  (  segid "BrD " and resid 81   and name HG2%)
    3 600     3 200     1 900 peak 27332 weight  0 10000E+01 volume  0 35670E+02 ppm1      2 338 ppm2      0 758
OR {27332}
  (( segid "BrD " and resid 22   and name HG  ))
  (  segid "BrD " and resid 78   and name HD1%)
ASSI {27462}
  (  segid "BrD " and resid 22   and name HD1%)
  (( segid "BrD " and resid 25   and name HB  ))
    3 800     3 600     1 700 peak 27462 weight  0 10000E+01 volume  0 26281E+02 ppm1      1.648 ppm2      2.995
OR {27462}
  (  segid "BrD " and resid 22   and name HD1%)
  (( segid "BrD " and resid 61   and name HG1 ))
OR {27462}
  (  segid "BrD " and resid 22   and name HD1%)
  (( segid "BrD " and resid 74   and name HB2 ))
ASSI {27482}
  (  segid "BrD " and resid 22   and name HD2%)
  (( segid "BrD " and resid 26   and name HA  ))
    3 200     2 600     2 300 peak 27482 weight  0 10000E+01 volume  0 77977E+02 ppm1      1 599 ppm2      4 492
OR {27482}
  (  segid "BrD " and resid 22   and name HD2%)
  (( segid "BrD " and resid 58   and name HA  ))
ASSI {27502}
  (  segid "BrD " and resid 22   and name HD2%)
  (( segid "BrD " and resid 59   and name HA  ))
    3 200     2 600     2.300 peak 27502 weight  0.10000E+01 volume  0 74913E+02 ppm1      1 599 ppm2      4 901
OR {27502}
  (  segid "BrD " and resid 22   and name HD2%)
  (( segid "BrD " and resid 35   and name HA  ))
OR {27502}
  (  segid "BrD " and resid 22   and name HD2%)
  (( segid "BrD " and resid 20   and name HA  ))
ASSI {27542}
  (  segid "BrD " and resid 22   and name HD2%)
  (( segid "BrD " and resid 56   and name HB2 ))
    4 000     4 000     1.500 peak 27542 weight  0.10000E+01 volume  0 19846E+02 ppm1      1.599 ppm2      2.011
OR {27542}
  (  segid "BrD " and resid 22   and name HD2%)
  (( segid "BrD " and resid 81   and name HB  ))
ASSI {27562}
  (  segid "BrD " and resid 22   and name HD1%)
  (( segid "BrD " and resid 64   and name HA  ))
    3 300     2 700     2 200 peak 27562 weight  0 10000E+01 volume  0.62753E+02 ppm1      1 645 ppm2      4 911
OR {27562}
  (  segid "BrD " and resid 22   and name HD1%)
  (( segid "BrD " and resid 59   and name HA  ))
ASSI {27592}
  (( segid "BrD " and resid 110  and name HG12))
  (  segid "BrD " and resid 115  and name HD1%)
    3 300     2 700     2 200 peak 27592 weight  0 10000E+01 volume  0 61111E+02 ppm1      1 646 ppm2      1 321
OR {27592}
  (( segid "BrD " and resid 110  and name HG12))
  (( segid "BrD " and resid 78   and name HB1 ))
OR {27592}
  (  segid "BrD " and resid 22   and name HD1%)
  (  segid "BrD " and resid 102  and name HD2%)
OR {27592}
  (( segid "BrD " and resid 110  and name HG12))
  (  segid "BrD " and resid 102  and name HD2%)
ASSI {27622}
  (  segid "BrD " and resid 73   and name HD2%)
  (( segid "BrD " and resid 74   and name HA  ))
    3 000     2 200     2 200 peak 27622 weight  0 10000E+01 volume  0 10007E+03 ppm1      1 500 ppm2      4 362
OR {27622}
  (  segid "BrD " and resid 73   and name HD2%)
  (( segid "BrD " and resid 70   and name HB2 ))
ASSI {27832}
  (( segid "BrD " and resid 78   and name HA  ))
  (( segid "BrD " and resid 82   and name HZ  ))
    3.500     3 100     2 000 peak 27832 weight  0 10000E+01 volume  0.44344E+02 ppm1      3 966 ppm2      7 023
OR {27832}
  (( segid "BrD " and resid 78   and name HA  ))
  (  segid "BrD " and resid 74   and name HD% )
ASSI {27852}
  (( segid "BrD " and resid 78   and name HB2 ))
  (( segid "BrD " and resid 116  and name HG12))
    4 700     4.700     0 800 peak 27852 weight  0 10000E+01 volume  0 74355E+01 ppm1      1 056 ppm2      1 531
OR {27852}
  (( segid "BrD " and resid 78   and name HB2 ))
  (  segid "BrD " and resid 56   and name HD1%)
ASSI {27862}
  (( segid "BrD " and resid 78   and name HB2 ))
  (( segid "BrD " and resid 110  and name HG12))
    3 700     3 400     1 800 peak 27862 weight  0 10000E+01 volume  0 33112E+02 ppm1      1 054 ppm2      1 629
OR {27862}
  (( segid "BrD " and resid 78   and name HB2 ))
  (  segid "BrD " and resid 21   and name HG2%)
OR {27862}
  (( segid "BrD " and resid 78   and name HB2 ))
  (  segid "BrD " and resid 22   and name HD2%)
OR {27862}
  (( segid "BrD " and resid 78   and name HB2 ))
  (( segid "BrD " and resid 21   and name HG12))
ASSI {27962}
  (  segid "BrD " and resid 78   and name HD1%)
  (  segid "BrD " and resid 74   and name HD% )
    2 200     2.200     2 300 peak 27962 weight  0.10000E+01 volume  0 80433E+03 ppm1      0 761 ppm2      7 031
OR {27962}
  (  segid "BrD " and resid 78   and name HD1%)
  (  segid "BrD " and resid 82   and name HE% )
ASSI {28022}
  (  segid "BrD " and resid 78   and name HD2%)
  (( segid "BrD " and resid 22   and name HA  ))
    3 100     2 400     2 400 peak 28022 weight  0 10000E+01 volume  0 92248E+02 ppm1      0.662 ppm2      4 727
OR {28022}
  (  segid "BrD " and resid 78   and name HD2%)
  (( segid "BrD " and resid 82   and name HA  ))
ASSI {28042}
  (  segid "BrD " and resid 78   and name HD2%)
  (( segid "BrD " and resid 56   and name HA  ))
    3.600     3 200     1 900 peak 28042 weight  0.10000E+01 volume  0.33967E+02 ppm1      0 662 ppm2      4 631
OR {28042}
  (  segid "BrD " and resid 78   and name HD2%)
  (( segid "BrD " and resid 76   and name HA  ))
OR {28042}
  (  segid "BrD " and resid 78   and name HD2%)
  (( segid "BrD " and resid 80   and name HA  ))
OR {28042}
  (  segid "BrD " and resid 78   and name HD2%)
  (( segid "BrD " and resid 104  and name HA  ))
OR {28042}
  (  segid "BrD " and resid 78   and name HD2%)
  (( segid "BrD " and resid 20   and name HB1 ))
OR {28042}
  (  segid "BrD " and resid 78   and name HD2%)
  (( segid "BrD " and resid 109  and name HA  ))
OR {28042}
  (  segid "BrD " and resid 78   and name HD2%)
  (( segid "BrD " and resid 14   and name HA  ))
OR {28042}
  (  segid "BrD " and resid 78   and name HD2%)
  (( segid "BrD " and resid 71   and name HA  ))
OR {28042}
  (  segid "BrD " and resid 78   and name HD2%)
  (( segid "BrD " and resid 15   and name HA  ))
ASSI {28052}
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  ( segid "BrD " and resid 78   and name HD1%)
  (( segid "BrD " and resid 56   and name HA  ))
    3.800     3.600     1 700 peak 28052 weight  0 10000E+01 volume  0 28600E+02 ppm1      0 761 ppm2       4 631
OR {28052}
  ( segid "BrD " and resid 78   and name HD1%)
  (( segid "BrD " and resid 76   and name HA  ))
OR {28052}
  ( segid "BrD " and resid 78   and name HD1%)
  (( segid "BrD " and resid 80   and name HA  ))
OR {28052}
  ( segid "BrD " and resid 78   and name HD1%)
  (( segid "BrD " and resid 60   and name HB2 ))
ASSI {28072}
  ( segid "BrD " and resid 78   and name HD1%)
  (( segid "BrD " and resid 79   and name HA  ))
    3 400     2 900     2 100 peak 28072 weight  0 10000E+01 volume  0 48389E+02 ppm1      0 761 ppm2       4.428
OR {28072}
  ( segid "BrD " and resid 78   and name HD1%)
  (( segid "BrD " and resid 25   and name HA  ))
OR {28072}
  ( segid "BrD " and resid 78   and name HD1%)
  (( segid "BrD " and resid 107  and name HA  ))
OR {28072}
  ( segid "BrD " and resid 78   and name HD1%)
  (( segid "BrD " and resid 99   and name HA  ))
ASSI {28082}
  ( segid "BrD " and resid 78   and name HD2%)
  (( segid "BrD " and resid 106  and name HA  ))
    3.000     2 200     2 200 peak 28082 weight  0 10000E+01 volume  0 10774E+03 ppm1      0 662 ppm2       4 525
OR {28082}
  ( segid "BrD " and resid 78   and name HD2%)
  (( segid "BrD " and resid 75   and name HA  ))
ASSI {28092}
  ( segid "BrD " and resid 78   and name HD2%)
  (( segid "BrD " and resid 79   and name HA  ))
    2.900     2 100     2 100 peak 28092 weight  0 10000E+01 volume  0 12398E+03 ppm1      0 662 ppm2       4.427
OR {28092}
  ( segid "BrD " and resid 78   and name HD2%)
  (( segid "BrD " and resid 107  and name HA  ))
ASSI {28112}
  ( segid "BrD " and resid 78   and name HD1%)
  (( segid "BrD " and resid 106  and name HB2 ))
    3 200     2 600     2 300 peak 28112 weight  0 10000E+01 volume  0 76864E+02 ppm1      0 760 ppm2       3 711
OR {28112}
  ( segid "BrD " and resid 78   and name HD1%)
  (( segid "BrD " and resid 81   and name HA  ))
ASSI {28142}
  ( segid "BrD " and resid 78   and name HD2%)
  (( segid "BrD " and resid 25   and name HB  ))
    3 900     3 800     1 600 peak 28142 weight  0 10000E+01 volume  0 22598E+02 ppm1      0 662 ppm2       3 005
OR {28142}
  ( segid "BrD " and resid 78   and name HD2%)
  (( segid "BrD " and resid 79   and name HG1 ))
OR {28142}
  ( segid "BrD " and resid 78   and name HD2%)
  (( segid "BrD " and resid 74   and name HB2 ))
ASSI {28152}
  ( segid "BrD " and resid 78   and name HD2%)
  (( segid "BrD " and resid 21   and name HG11))
    3 600     3 200     1 900 peak 28152 weight  0.10000E+01 volume  0 38156E+02 ppm1      0.662 ppm2       2.347
OR {28152}
  ( segid "BrD " and resid 78   and name HD2%)
  (( segid "BrD " and resid 56   and name HG  ))
OR {28152}
  ( segid "BrD " and resid 78   and name HD2%)
  (( segid "BrD " and resid 22   and name HG  ))
ASSI {28162}
  ( segid "BrD " and resid 78   and name HD2%)
  ( segid "BrD " and resid 75   and name HE% )
    4 300     4 300     1 200 peak 28162 weight  0 10000E+01 volume  0 12997E+02 ppm1      0 662 ppm2       2.670
OR {28162}
  ( segid "BrD " and resid 78   and name HD2%)
  (( segid "BrD " and resid 79   and name HB2 ))
OR {28162}
  ( segid "BrD " and resid 78   and name HD2%)
  (( segid "BrD " and resid 22   and name HB1 ))
ASSI {28172}
  ( segid "BrD " and resid 78   and name HD1%)
  (( segid "BrD " and resid 74   and name HB2 ))
    3 800     3 600     1 700 peak 28172 weight  0.10000E+01 volume  0 27394E+02 ppm1      0 760 ppm2       3 003
OR {28172}
  ( segid "BrD " and resid 78   and name HD1%)
  (( segid "BrD " and resid 25   and name HB  ))
ASSI {28302}
  ( segid "BrD " and resid 56   and name HD2%)
  (( segid "BrD " and resid 35   and name HA  ))
    2.600     1.700     1 700 peak 28302 weight  0 10000E+01 volume  0 27298E+03 ppm1      1 254 ppm2       4 907
OR {28302}
  ( segid "BrD " and resid 56   and name HD2%)
  (( segid "BrD " and resid 59   and name HA  ))
ASSI {28332}
  ( segid "BrD " and resid 56   and name HD2%)
  (( segid "BrD " and resid 25   and name HA  ))
    5 000     5 000     0 500 peak 28332 weight  0 10000E+01 volume  0 51532E+01 ppm1      1 253 ppm2       4 441
OR {28332}
  ( segid "BrD " and resid 56   and name HD2%)
  (( segid "BrD " and resid 58   and name HA  ))
ASSI {28482}
  (( segid "BrD " and resid 56   and name HB2 ))
  ( segid "BrD " and resid 81   and name HG2%)
    3 700     3 400     1 800 peak 28482 weight  0 10000E+01 volume  0 33282E+02 ppm1      1 993 ppm2       0.766
OR {28482}
  (( segid "BrD " and resid 102  and name HB1 ))
  ( segid "BrD " and resid 81   and name HG2%)
ASSI {28552}
  (( segid "BrD " and resid 102  and name HG  ))
  (( segid "BrD " and resid 25   and name HA  ))
    4 000     4 000     1 500 peak 28552 weight  0 10000E+01 volume  0 18876E+02 ppm1      2 141 ppm2       4 445
OR {28552}
  (( segid "BrD " and resid 102  and name HG  ))
  (( segid "BrD " and resid 99   and name HA  ))
OR {28552}
  (( segid "BrD " and resid 97   and name HG2 ))
  (( segid "BrD " and resid 96   and name HA  ))
ASSI {28592}
  ( segid "BrD " and resid 102  and name HD2%)
  (( segid "BrD " and resid 34   and name HZ  ))
    3 700     3.400     1 800 peak 28592 weight  0 10000E+01 volume  0 30371E+02 ppm1      1 303 ppm2       7 899
OR {28592}
  ( segid "BrD " and resid 102  and name HD2%)
  ( segid "BrD " and resid 107  and name HE% )
ASSI {28602}
  ( segid "BrD " and resid 102  and name HD2%)
  ( segid "BrD " and resid 34   and name HE% )
    2 000     2 000     2.500 peak 28602 weight  0 10000E+01 volume  0 10851E+04 ppm1      1 303 ppm2       7 771
OR {28602}
  ( segid "BrD " and resid 102  and name HD2%)
  ( segid "BrD " and resid 105  and name HD% )
ASSI {28682}
  ( segid "BrD " and resid 102  and name HD1%)
  (( segid "BrD " and resid 28   and name HA  ))
    4 000     4 000     1 500 peak 28682 weight  0 10000E+01 volume  0 20825E+02 ppm1      1 303 ppm2       4 581
OR {28682}
  ( segid "BrD " and resid 102  and name HD1%)
  (( segid "BrD " and resid 106  and name HA  ))
ASSI {28692}
  ( segid "BrD " and resid 102  and name HD1%)
  (( segid "BrD " and resid 30   and name HB2 ))
    2.700     1.800     1 800 peak 28692 weight  0 10000E+01 volume  0 20830E+03 ppm1      1 303 ppm2       4 526
OR {28692}
  ( segid "BrD " and resid 102  and name HD1%)
  (( segid "BrD " and resid 28   and name HA  ))
ASSI {28772}
  ( segid "BrD " and resid 102  and name HD2%)
  ( segid "BrD " and resid 78   and name HD1%)
    3 500     3 100     2 000 peak 28772 weight  0 10000E+01 volume  0 44195E+02 ppm1      1 304 ppm2       0 760
OR {28772}
  ( segid "BrD " and resid 102  and name HD2%)
  ( segid "BrD " and resid 81   and name HG2%)
ASSI {28862}
  (( segid "BrD " and resid 115  and name HB1 ))
  (( segid "BrD " and resid 110  and name HG11))
    3 300     2 700     2 200 peak 28862 weight  0 10000E+01 volume  0 61541E+02 ppm1      2 190 ppm2       1 742
OR {28862}
  (( segid "BrD " and resid 115  and name HB1 ))
  ( segid "BrD " and resid 17   and name HG2%)
ASSI {28952}
  ( segid "BrD " and resid 56   and name HD1%)
  (( segid "BrD " and resid 31   and name HA  ))
    3 100     2 400     2 400 peak 28952 weight  0 10000E+01 volume  0 92579E+02 ppm1      1 548 ppm2       4 984
OR {28952}
  ( segid "BrD " and resid 56   and name HD1%)
  (( segid "BrD " and resid 60   and name HB1 ))
ASSI {29002}
  ( segid "BrD " and resid 59   and name HE% )
  ( segid "BrD " and resid 76   and name HB% )
    3.500     3 100     2.000 peak 29002 weight  0 10000E+01 volume  0 43704E+02 ppm1      1 848 ppm2       2 108
OR {29002}
  ( segid "BrD " and resid 59   and name HE% )
  (( segid "BrD " and resid 18   and name HB1 ))
OR {29002}
  ( segid "BrD " and resid 59   and name HE% )
  (( segid "BrD " and resid 102  and name HG  ))
ASSI {29022}
  ( segid "BrD " and resid 59   and name HE% )
  (( segid "BrD " and resid 22   and name HB2 ))
    3.400     2.900     2 100 peak 29022 weight  0 10000E+01 volume  0 52140E+02 ppm1      1 848 ppm2       2 292
OR {29022}
  ( segid "BrD " and resid 59   and name HE% )
  (( segid "BrD " and resid 18   and name HG  ))
OR {29022}
  ( segid "BrD " and resid 59   and name HE% )
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  ( segid "BrD " and resid 31   and name HB% )
ASSI {29032}
  ( segid "BrD " and resid 59   and name HE% )
  (( segid "BrD " and resid 56   and name HG  ))
    3.700     3 400     1 800 peak 29032 weight  0.10000E+01 volume  0 29631E+02 ppm1      1 848 ppm2      2 361
OR {29032}
  ( segid "BrD " and resid 59   and name HE% )
  (( segid "BrD " and resid 22   and name HG  ))
OR {29032}
  ( segid "BrD " and resid 59   and name HE% )
  (( segid "BrD " and resid 73   and name HG  ))
OR {29032}
  ( segid "BrD " and resid 59   and name HE% )
  (( segid "BrD " and resid 21   and name HG11))
ASSI {29072}
  ( segid "BrD " and resid 59   and name HE% )
  (( segid "BrD " and resid 22   and name HA  ))
    4.200     4 200     1 300 peak 29072 weight  0 10000E+01 volume  0 14615E+02 ppm1      1 848 ppm2      4 719
OR {29072}
  ( segid "BrD " and resid 59   and name HE% )
  (( segid "BrD " and resid 58   and name HB  ))
OR {29072}
  ( segid "BrD " and resid 59   and name HE% )
  (( segid "BrD " and resid 69   and name HA  ))
OR {29072}
  ( segid "BrD " and resid 59   and name HE% )
  (( segid "BrD " and resid 53   and name HA  ))
ASSI {29152}
  ( segid "BrD " and resid 59   and name HE% )
  ( segid "BrD " and resid 73   and name HD2%)
    3 600     3 200     1 900 peak 29152 weight  0 10000E+01 volume  0 38252E+02 ppm1      1 848 ppm2      1 462
OR {29152}
  ( segid "BrD " and resid 59   and name HE% )
  ( segid "BrD " and resid 63   and name HD2%)
OR {29152}
  ( segid "BrD " and resid 59   and name HE% )
  (( segid "BrD " and resid 62   and name HG2 ))
ASSI {29192}
  ( segid "BrD " and resid 54   and name HE% )
  (( segid "BrD " and resid 60   and name HB1 ))
    3.200     2.600     2 300 peak 29192 weight  0 10000E+01 volume  0 76364E+02 ppm1      2 536 ppm2      4 964
OR {29192}
  ( segid "BrD " and resid 54   and name HE% )
  (( segid "BrD " and resid 77   and name HA  ))
ASSI {29202}
  ( segid "BrD " and resid 54   and name HE% )
  (( segid "BrD " and resid 55   and name HB1 ))
    3 700     3 400     1 800 peak 29202 weight  0 10000E+01 volume  0.30281E+02 ppm1      2 535 ppm2      2 955
OR {29202}
  ( segid "BrD " and resid 54   and name HE% )
  (( segid "BrD " and resid 37   and name HB1 ))
ASSI {29252}
  ( segid "BrD " and resid 54   and name HE% )
  ( segid "BrD " and resid 35   and name HE% )
    2 500     2 500     2 000 peak 29252 weight  0.10000E+01 volume  0 29954E+03 ppm1      2 535 ppm2      2 801
OR {29252}
  ( segid "BrD " and resid 54   and name HE% )
  (( segid "BrD " and resid 53   and name HB1 ))
OR {29252}
  ( segid "BrD " and resid 54   and name HE% )
  (( segid "BrD " and resid 61   and name HG2 ))
OR {29252}
  ( segid "BrD " and resid 54   and name HE% )
  (( segid "BrD " and resid 36   and name HG1 ))
ASSI {29262}
  ( segid "BrD " and resid 54   and name HE% )
  (( segid "BrD " and resid 37   and name HG1 ))
    2 600     1 700     1 700 peak 29262 weight  0.10000E+01 volume  0 23100E+03 ppm1      2 535 ppm2      2 722
OR {29262}
  ( segid "BrD " and resid 54   and name HE% )
  (( segid "BrD " and resid 59   and name HB1 ))
ASSI {29582}
  (( segid "BrD " and resid 79   and name HA  ))
  (( segid "BrD " and resid 116  and name HG11))
    4 100     4 100     1.400 peak 29582 weight  0 10000E+01 volume  0 16991E+02 ppm1      4.409 ppm2      1 897
OR {29582}
  (( segid "BrD " and resid 79   and name HA  ))
  (( segid "BrD " and resid 103  and name HB2 ))
ASSI {29682}
  (( segid "BrD " and resid 108  and name HA  ))
  (( segid "BrD " and resid 111  and name HG1 ))
    4 100     4.100     1 400 peak 29682 weight  0 10000E+01 volume  0 16470E+02 ppm1      4 804 ppm2      2.003
OR {29682}
  (( segid "BrD " and resid 108  and name HA  ))
  (( segid "BrD " and resid 109  and name HD1 ))
ASSI {29702}
  (( segid "BrD " and resid 15   and name HA  ))
  (( segid "BrD " and resid 19   and name HB2 ))
    2 800     2 000     2 000 peak 29702 weight  0.10000E+01 volume  0 16053E+03 ppm1      4.607 ppm2      1 986
OR {29702}
  (( segid "BrD " and resid 108  and name HB1 ))
  (( segid "BrD " and resid 109  and name HD1 ))
OR {29702}
  (( segid "BrD " and resid 60   and name HB2 ))
  (( segid "BrD " and resid 56   and name HB2 ))
ASSI {29712}
  (( segid "BrD " and resid 15   and name HA  ))
  (( segid "BrD " and resid 18   and name HB1 ))
    3 100     2 400     2.400 peak 29712 weight  0 10000E+01 volume  0.92305E+02 ppm1      4 607 ppm2      2 182
OR {29712}
  (( segid "BrD " and resid 60   and name HB2 ))
  (( segid "BrD " and resid 64   and name HG1 ))
ASSI {29722}
  (( segid "BrD " and resid 15   and name HA  ))
  ( segid "BrD " and resid 14   and name HD2%)
    3.900     3 800     1 600 peak 29722 weight  0 10000E+01 volume  0.22638E+02 ppm1      4 607 ppm2      1 417
OR {29722}
  (( segid "BrD " and resid 15   and name HA  ))
  ( segid "BrD " and resid 69   and name HG2%)
ASSI {29732}
  (( segid "BrD " and resid 30   and name HA  ))
  (( segid "BrD " and resid 98   and name HA  ))
    2 600     1.700     1.700 peak 29732 weight  0 10000E+01 volume  0 26724E+03 ppm1      5.445 ppm2      4 810
OR {29732}
  (( segid "BrD " and resid 30   and name HA  ))
  (( segid "BrD " and resid 29   and name HA  ))
ASSI {30592}
  (( segid "BrD " and resid 109  and name HB1 ))
  ( segid "BrD " and resid 21   and name HD1%)
    3.700     3.400     1 800 peak 30592 weight  0 10000E+01 volume  0 31262E+02 ppm1      2 334 ppm2      1 222
OR {30592}
  (( segid "BrD " and resid 109  and name HB1 ))
  ( segid "BrD " and resid 110  and name HG2%)
ASSI {30672}
  (( segid "BrD " and resid 109  and name HB2 ))
  (( segid "BrD " and resid 110  and name HA  ))
    3.600     3 200     1 900 peak 30672 weight  0 10000E+01 volume  0 39278E+02 ppm1      2 141 ppm2      4 378
OR {30672}
  (( segid "BrD " and resid 109  and name HB2 ))
  (( segid "BrD " and resid 107  and name HA  ))
ASSI {30952}
  (( segid "BrD " and resid 75   and name HA  ))
  (( segid "BrD " and resid 78   and name HG  ))
    3 800     3 600     1 700 peak 30952 weight  0 10000E+01 volume  0.28077E+02 ppm1      4.509 ppm2      1 260
OR {30952}
  (( segid "BrD " and resid 26   and name HA  ))
  ( segid "BrD " and resid 56   and name HD2%)
ASSI {   83}
  ( segid "BrD " and resid 46   and name HD% )
  (( segid "BrD " and resid 47   and name HA  ))
    2 300     2 300     2 200 peak    83 weight  0 10000E+01 volume  0 20163E+03 ppm1      5 758 ppm2      4.693
OR {   83}
  ( segid "BrD " and resid 46   and name HD% )
  (( segid "BrD " and resid 53   and name HA  ))
ASSI {  533}
  ( segid "BrD " and resid 47   and name HE% )
  (( segid "BrD " and resid 38   and name HB  ))
    3 200     2 600     2 300 peak   533 weight  0.10000E+01 volume  0.34245E+02 ppm1      7 246 ppm2      1.776
OR {  533}
  ( segid "BrD " and resid 47   and name HE% )
  (( segid "BrD " and resid 50   and name HB  ))
ASSI {  643}
  ( segid "BrD " and resid 74   and name HD% )
  (( segid "BrD " and resid 71   and name HA  ))
    3 100     2 400     2 400 peak   643 weight  0 10000E+01 volume  0 35398E+02 ppm1      7 012 ppm2      4 622
OR {  643}
  ( segid "BrD " and resid 74   and name HD% )
  (( segid "BrD " and resid 15   and name HA  ))
OR {  643}
  ( segid "BrD " and resid 74   and name HD% )
  (( segid "BrD " and resid 76   and name HA  ))
OR {  643}
  ( segid "BrD " and resid 74   and name HD% )
  (( segid "BrD " and resid 56   and name HA  ))
OR {  643}
  ( segid "BrD " and resid 74   and name HD% )
  (( segid "BrD " and resid 72   and name HA  ))
OR {  643}
  ( segid "BrD " and resid 74   and name HD% )
  (( segid "BrD " and resid 14   and name HA  ))
ASSI { 1143}
  ( segid "BrD " and resid 105  and name HD% )
  ( segid "BrD " and resid 101  and name HG2%)
    3 100     2 400     2 400 peak  1143 weight  0.10000E+01 volume  0 36890E+02 ppm1      7 758 ppm2      1 631
OR { 1143}
  ( segid "BrD " and resid 105  and name HD% )
  ( segid "BrD " and resid 21   and name HG2%)
ASSI { 1393}
  ( segid "BrD " and resid 96   and name HD% )
  (( segid "BrD " and resid 86   and name HA  ))
    2.200     2 200     2.300 peak  1393 weight  0 10000E+01 volume  0 26898E+03 ppm1      7.711 ppm2      4 810
OR { 1393}
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  ( segid "BrD " and resid 96   and name HD% )
  (( segid "BrD " and resid 92   and name HA  ))
ASSI { 1763}
  ( segid "BrD " and resid 106  and name HE% )
  (( segid "BrD " and resid 107  and name HA  ))
   3 400     2 900     2.100 peak  1763 weight  0 10000E+01 volume  0 21871E+02 ppm1     7 617 ppm2      4 431
OR { 1763}
  ( segid "BrD " and resid 106  and name HE% )
  (( segid "BrD " and resid 79   and name HA  ))
OR { 1763}
  ( segid "BrD " and resid 106  and name HE% )
  (( segid "BrD " and resid 110  and name HA  ))
ASSI { 1783}
  ( segid "BrD " and resid 106  and name HE% )
  ( segid "BrD " and resid 74   and name HD% )
   3 700     3 400     1 800 peak  1783 weight  0 10000E+01 volume  0 13872E+02 ppm1     7 617 ppm2      7 027
OR { 1783}
  ( segid "BrD " and resid 106  and name HE% )
  ( segid "BrD " and resid 82   and name HE% )
OR { 1783}
  ( segid "BrD " and resid 106  and name HE% )
  (( segid "BrD " and resid 82   and name HZ  ))
ASSI { 1813}
  ( segid "BrD " and resid 95   and name HD% )
  (( segid "BrD " and resid 94   and name HA  ))
   3 300     2 700     2.200 peak  1813 weight  0 10000E+01 volume  0 28141E+02 ppm1     7.478 ppm2      4 810
OR { 1813}
  ( segid "BrD " and resid 95   and name HD% )
  (( segid "BrD " and resid 86   and name HA  ))
ASSI { 1893}
  ( segid "BrD " and resid 96   and name HE% )
  (( segid "BrD " and resid 96   and name HA  ))
   3 600     3 200     1 900 peak  1893 weight  0 10000E+01 volume  0 14793E+02 ppm1     7 618 ppm2      4 387
OR { 1893}
  ( segid "BrD " and resid 95   and name HE% )
  (( segid "BrD " and resid 33   and name HA  ))
ASSI { 2063}
  (( segid "BrD " and resid 32   and name HZ3 ))
  (( segid "BrD " and resid 32   and name HA  ))
   5 500     5 500     0.000 peak  2063 weight  0 10000E+01 volume  0 11153E-03 ppm1     7 804 ppm2      4 971
OR { 2063}
  (( segid "BrD " and resid 32   and name HZ3 ))
  (( segid "BrD " and resid 93   and name HB1 ))
OR { 2063}
  (( segid "BrD " and resid 32   and name HZ3 ))
  (( segid "BrD " and resid 85   and name HA  ))
ASSI {   24}
  ( segid "BrD " and resid 46   and name HE% )
  (( segid "BrD " and resid 50   and name HB  ))
   3 600     3 200     1 900 peak    24 weight  0 10000E+01 volume  0 55296E+02 ppm1     6 687 ppm2      1 777
OR {   24}
  ( segid "BrD " and resid 46   and name HE% )
  (( segid "BrD " and resid 38   and name HB  ))
ASSI {   94}
  ( segid "BrD " and resid 82   and name HD% )
  (( segid "BrD " and resid 79   and name HA  ))
   2.200     1 200     1 200 peak    94 weight  0 10000E+01 volume  0 10359E+04 ppm1     7 266 ppm2      4.424
OR {   94}
  ( segid "BrD " and resid 82   and name HD% )
  (( segid "BrD " and resid 99   and name HA  ))
ASSI {  104}
  ( segid "BrD " and resid 47   and name HE% )
  (( segid "BrD " and resid 53   and name HG2 ))
   2 500     1 600     1 600 peak   104 weight  0 10000E+01 volume  0 51584E+03 ppm1     7 270 ppm2      2.504
OR {  104}
  ( segid "BrD " and resid 82   and name HD% )
  (( segid "BrD " and resid 103  and name HG2 ))
ASSI {  124}
  ( segid "BrD " and resid 47   and name HD% )
  (( segid "BrD " and resid 50   and name HG12))
   3 600     3 200     1 900 peak   124 weight  0 10000E+01 volume  0 55730E+02 ppm1     7 970 ppm2      0 780
OR {  124}
  ( segid "BrD " and resid 47   and name HD% )
  ( segid "BrD " and resid 38   and name HG2%)
ASSI {  134}
  ( segid "BrD " and resid 47   and name HD% )
  (( segid "BrD " and resid 53   and name HD2 ))
   2.900     2 100     2 100 peak   134 weight  0 10000E+01 volume  0 18431E+03 ppm1     7 970 ppm2      4 007
OR {  134}
  (( segid "BrD " and resid 32   and name HZ2 ))
  (( segid "BrD " and resid 98   and name HB1 ))
ASSI {  554}
  (( segid "BrD " and resid 28   and name HE1 ))
  (( segid "BrD " and resid 30   and name HB2 ))
   2 900     2 100     2 100 peak   554 weight  0.10000E+01 volume  0 21924E+03 ppm1     8 158 ppm2      4.538
OR {  554}
  (( segid "BrD " and resid 28   and name HE1 ))
  (( segid "BrD " and resid 28   and name HA  ))
ASSI {  574}
  ( segid "BrD " and resid 68   and name HE% )
  (( segid "BrD " and resid 59   and name HA  ))
   3.200     2.600     2.300 peak   574 weight  0.10000E+01 volume  0.10500E+03 ppm1     7.921 ppm2      4.930
OR {  574}
  (( segid "BrD " and resid 32   and name HE3 ))
  (( segid "BrD " and resid 32   and name HA  ))
ASSI {  604}
  (( segid "BrD " and resid 107  and name HZ  ))
  (( segid "BrD " and resid 83   and name HB  ))
   3 500     3 100     2 000 peak   604 weight  0 10000E+01 volume  0 65660E+02 ppm1     8 063 ppm2      4 784
OR {  604}
  (( segid "BrD " and resid 107  and name HZ  ))
  (( segid "BrD " and resid 82   and name HA  ))
ASSI {  614}
  (( segid "BrD " and resid 107  and name HZ  ))
  (( segid "BrD " and resid 80   and name HA  ))
   3.300     2 700     2 200 peak   614 weight  0.10000E+01 volume  0.96219E+02 ppm1     8.062 ppm2      4 673
OR {  614}
  (( segid "BrD " and resid 107  and name HZ  ))
  (( segid "BrD " and resid 118  and name HA  ))
OR {  614}
  (( segid "BrD " and resid 107  and name HZ  ))
  (( segid "BrD " and resid 76   and name HA  ))
ASSI {  704}
  (( segid "BrD " and resid 107  and name HZ  ))
  (( segid "BrD " and resid 79   and name HB1 ))
   2 800     2 000     2 000 peak   704 weight  0 10000E+01 volume  0.25291E+03 ppm1     8.009 ppm2      2 755
OR {  704}
  (( segid "BrD " and resid 32   and name HZ2 ))
  (( segid "BrD " and resid 94   and name HB1 ))
ASSI {  794}
  (( segid "BrD " and resid 32   and name HE3 ))
  (( segid "BrD " and resid 32   and name HB2 ))
   2 600     1 700     1 700 peak   794 weight  0 10000E+01 volume  0 39954E+03 ppm1     7 960 ppm2      4 212
OR {  794}
  ( segid "BrD " and resid 47   and name HD% )
  (( segid 'BrD   and resid 53   and name HD1 ))
ASSI {  964}
  (( segid "BrD " and resid 34   and name HZ  ))
  (( segid "BrD " and resid 28   and name HD2 ))
   4 200     4 200     1 300 peak   964 weight  0.10000E+01 volume  0 22395E+02 ppm1     7 928 ppm2      5.579
OR {  964}
  (( segid "BrD " and resid 34   and name HZ  ))
  (( segid "BrD " and resid 34   and name HA  ))
ASSI {  974}
  (( segid "BrD " and resid 34   and name HZ  ))
  (( segid "BrD " and resid 98   and name HA  ))
   3 800     3 600     1 700 peak   974 weight  0.10000E+01 volume  0 41681E+02 ppm1     7 929 ppm2      4.791
OR {  974}
  (( segid "BrD " and resid 34   and name HZ  ))
  (( segid "BrD " and resid 82   and name HA  ))
ASSI { 1044}
  ( segid "BrD " and resid 107  and name HE% )
  (( segid "BrD " and resid 79   and name HA  ))
   2.300     1.300     1 300 peak  1044 weight  0 10000E+01 volume  0.88364E+03 ppm1     7.921 ppm2      4.440
OR { 1044}
  (( segid "BrD " and resid 34   and name HZ  ))
  (( segid "BrD " and resid 99   and name HA  ))
ASSI { 1074}
  (( segid "BrD " and resid 34   and name HZ  ))
  ( segid "BrD " and resid 102  and name HD1%)
   2 900     2.100     2.100 peak  1074 weight  0 10000E+01 volume  0 20962E+03 ppm1     7 924 ppm2      1.333
OR { 1074}
  ( segid "BrD " and resid 107  and name HE% )
  (( segid "BrD " and resid 78   and name HB1 ))
ASSI { 1084}
  (( segid "BrD " and resid 34   and name HZ  ))
  (( segid "BrD " and resid 98   and name HA  ))
   4 000     4.000     1.500 peak  1084 weight  0 10000E+01 volume  0 28521E+02 ppm1     7 913 ppm2      4 791
OR { 1084}
  (( segid "BrD " and resid 34   and name HZ  ))
  (( segid "BrD " and resid 82   and name HA  ))
OR { 1084}
  ( segid "BrD " and resid 68   and name HE% )
  (( segid "BrD " and resid 73   and name HA  ))
ASSI { 1094}
  ( segid "BrD " and resid 107  and name HE% )
  (( segid "BrD " and resid 118  and name HA  ))
   3.200     2.600     2 300 peak  1094 weight  0 10000E+01 volume  0 10760E+03 ppm1     7.918 ppm2      4 683
OR { 1094}
  ( segid "BrD " and resid 107  and name HE% )
  (( segid "BrD " and resid 76   and name HA  ))
OR { 1094}
  ( segid "BrD " and resid 68   and name HE% )
  (( segid "BrD " and resid 58   and name HB  ))
OR { 1094}
  ( segid "BrD " and resid 68   and name HE% )
  (( segid "BrD " and resid 67   and name HA  ))
OR { 1094}
  ( segid "BrD " and resid 107  and name HE% )
  (( segid "BrD " and resid 104  and name HA  ))
OR { 1094}
  ( segid "BrD " and resid 107  and name HE% )
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  (( segid "BrD " and resid 80   and name HA  ))
OR ( 1094)
   (  segid "BrD " and resid 68   and name HE% )
   (( segid "BrD " and resid 69   and name HA  ))
ASSI ( 1104)
   (( segid "BrD " and resid 34   and name HZ  ))
   (  segid "BrD " and resid 99   and name HB% )
     2.400      1 400      1 400 peak  1104 weight  0 10000E+01 volume  0 63603E+03 ppm1      7 907 ppm2      2 212
OR ( 1104)
   (( segid "BrD " and resid 34   and name HZ  ))
   (( segid "BrD " and resid 33   and name HD2 ))
ASSI ( 1114)
   (  segid "BrD " and resid 68   and name HE% )
   (  segid "BrD " and resid 68   and name HD% )
     2 100      1 100      1 100 peak  1114 weight  0 10000E+01 volume  0 15242E+04 ppm1      7 904 ppm2      7 776
OR ( 1114)
   (  segid "BrD " and resid 107  and name HE% )
   (  segid "BrD " and resid 107  and name HD% )
OR ( 1114)
   (( segid "BrD " and resid 34   and name HZ  ))
   (  segid "BrD " and resid 34   and name HE% )
ASSI ( 1124)
   (( segid "BrD " and resid 34   and name HZ  ))
   (( segid "BrD " and resid 98   and name HB2 ))
     2.500      1 600      1 600 peak  1124 weight  0 10000E+01 volume  0 54441E+03 ppm1      7 898 ppm2      3 659
OR ( 1124)
   (  segid "BrD " and resid 107  and name HE% )
   (( segid "BrD " and resid 82   and name HB1 ))
OR ( 1124)
   (  segid "BrD " and resid 68   and name HE% )
   (( segid "BrD " and resid 68   and name HB1 ))
ASSI ( 1134)
   (  segid "BrD " and resid 68   and name HE% )
   (( segid "BrD " and resid 62   and name HG1 ))
     3 600      3 200      1 900 peak  1134 weight  0.10000E+01 volume  0 60159E+02 ppm1      7 900 ppm2      2 343
OR ( 1134)
   (  segid "BrD " and resid 68   and name HE% )
   (( segid "BrD " and resid 73   and name HG  ))
ASSI ( 1164)
   (  segid "BrD " and resid 68   and name HE% )
   (( segid "BrD " and resid 62   and name HG1 ))
     3 200      2.600      2.300 peak  1164 weight  0.10000E+01 volume  0.12306E+03 ppm1      7 896 ppm2      2 374
OR ( 1164)
   (  segid "BrD " and resid 68   and name HE% )
   (( segid "BrD " and resid 73   and name HG  ))
OR ( 1164)
   (  segid "BrD " and resid 107  and name HE% )
   (( segid "BrD " and resid 116  and name HB  ))
ASSI ( 1204)
   (  segid "BrD " and resid 68   and name HE% )
   (( segid "BrD " and resid 68   and name HB2 ))
     2 500      1.600      1 600 peak  1204 weight  0 10000E+01 volume  0 47618E+03 ppm1      7 892 ppm2      3 546
OR ( 1204)
   (  segid "BrD " and resid 68   and name HE% )
   (( segid "BrD " and resid 67   and name HB1 ))
OR ( 1204)
   (  segid "BrD " and resid 107  and name HE% )
   (( segid "BrD " and resid 82   and name HB2 ))
OR ( 1204)
   (( segid "BrD " and resid 34   and name HZ  ))
   (( segid "BrD " and resid 82   and name HB2 ))
ASSI ( 1244)
   (  segid "BrD " and resid 107  and name HE% )
   (( segid "BrD " and resid 79   and name HB2 ))
     2 500      1 600      1 600 peak  1244 weight  0 10000E+01 volume  0 54491E+03 ppm1      7 891 ppm2      2 644
OR ( 1244)
   (  segid "BrD " and resid 68   and name HE% )
   (( segid "BrD " and resid 62   and name HD2 ))
ASSI ( 1254)
   (  segid "BrD " and resid 107  and name HE% )
   (( segid "BrD " and resid 116  and name HG11))
     2.700      1 800      1.800 peak  1254 weight  0.10000E+01 volume  0 30083E+03 ppm1      7 891 ppm2      1 886
OR ( 1254)
   (  segid "BrD " and resid 68   and name HE% )
   (  segid "BrD " and resid 59   and name HE% )
OR ( 1254)
   (  segid "BrD " and resid 107  and name HE% )
   (( segid "BrD " and resid 103  and name HB2 ))
ASSI ( 1274)
   (( segid "BrD " and resid 34   and name HZ  ))
   (( segid "BrD " and resid 98   and name HA  ))
     3.400      2.900      2.100 peak  1274 weight  0 10000E+01 volume  0 84175E+02 ppm1      7.888 ppm2      4 815
OR ( 1274)
   (  segid "BrD " and resid 68   and name HE% )
   (( segid "BrD " and resid 73   and name HA  ))
ASSI ( 1284)
   (  segid "BrD " and resid 107  and name HE% )
   (( segid "BrD " and resid 103  and name HG2 ))
     2 500      1 600      1 600 peak  1284 weight  0 10000E+01 volume  0.45504E+03 ppm1      7 889 ppm2      2.554
OR ( 1284)
   (  segid "BrD " and resid 68   and name HE% )
  (( segid "BrD " and resid 54   and name HB1 ))
ASSI ( 1294)
   (  segid "BrD " and resid 107  and name HE% )
   (( segid "BrD " and resid 116  and name HB  ))
     3 300      2 700      2 200 peak  1294 weight  0 10000E+01 volume  0 10144E+03 ppm1      7.888 ppm2      2 422
OR ( 1294)
   (( segid "BrD " and resid 34   and name HZ  ))
   (( segid "BrD " and resid 101  and name HG11))
ASSI ( 1304)
   (  segid "BrD " and resid 68   and name HE% )
   (  segid "BrD " and resid 58   and name HG2%)
     2.600      1 700      1 700 peak  1304 weight  0 10000E+01 volume  0 38056E+03 ppm1      7 888 ppm2      1 656
OR ( 1304)
   (  segid "BrD " and resid 107  and name HE% )
   (( segid "BrD " and resid 110  and name HG12))
ASSI ( 1444)
   (  segid "BrD " and resid 107  and name HD% )
   (( segid "BrD " and resid 104  and name HA  ))
     2 900      2.100      2 100 peak  1444 weight  0 10000E+01 volume  0 19434E+03 ppm1      7 811 ppm2      4 684
OR ( 1444)
   (  segid "BrD " and resid 105  and name HD% )
   (( segid "BrD " and resid 104  and name HA  ))
OR ( 1444)
   (  segid "BrD " and resid 107  and name HD% )
   (( segid "BrD " and resid 118  and name HA  ))
OR ( 1444)
   (  segid "BrD " and resid 105  and name HD% )
   (( segid "BrD " and resid 109  and name HA  ))
ASSI ( 1504)
   (  segid "BrD " and resid 105  and name HD% )
   (( segid "BrD " and resid 105  and name HA  ))
     2 400      1 400      1.400 peak  1504 weight  0 10000E+01 volume  0 65395E+03 ppm1      7 798 ppm2      4 926
OR ( 1504)
   (  segid "BrD " and resid 68   and name HD% )
   (( segid "BrD " and resid 59   and name HA  ))
ASSI ( 1514)
   (  segid "BrD " and resid 107  and name HD% )
   (( segid "BrD " and resid 106  and name HA  ))
     2 800      2 000      2 000 peak  1514 weight  0 10000E+01 volume  0 27794E+03 ppm1      7 798 ppm2      4 572
OR ( 1514)
   (  segid "BrD " and resid 105  and name HD% )
   (( segid "BrD " and resid 106  and name HA  ))
OR ( 1514)
   (  segid "BrD " and resid 105  and name HD% )
   (( segid "BrD " and resid 108  and name HB1 ))
ASSI ( 1534)
   (  segid "BrD " and resid 105  and name HD% )
   (( segid "BrD " and resid 105  and name HB2 ))
     2 200      1 200      1 200 peak  1534 weight  0 10000E+01 volume  0 11824E+04 ppm1      7 799 ppm2      3 674
OR ( 1534)
   (  segid "BrD " and resid 107  and name HD% )
   (( segid "BrD " and resid 107  and name HB1 ))
OR ( 1534)
   (  segid "BrD " and resid 68   and name HD% )
   (( segid "BrD " and resid 68   and name HB1 ))
ASSI ( 1554)
   (  segid "BrD " and resid 34   and name HE% )
   (( segid "BrD " and resid 102  and name HB2 ))
     2 500      2 500      2 000 peak  1554 weight  0.10000E+01 volume  0 46212E+03 ppm1      7 799 ppm2      1 819
OR ( 1554)
   (  segid "BrD " and resid 68   and name HD% )
   (  segid "BrD " and resid 59   and name HE% )
ASSI ( 1574)
   (  segid "BrD " and resid 105  and name HD% )
   (( segid "BrD " and resid 102  and name HA  ))
     2 800      2 000      2.000 peak  1574 weight  0.10000E+01 volume  0 27340E+03 ppm1      7.797 ppm2      4.278
OR ( 1574)
   (  segid "BrD " and resid 105  and name HD% )
   (( segid "BrD " and resid 101  and name HA  ))
OR ( 1574)
   (  segid "BrD " and resid 34   and name HE% )
   (( segid "BrD " and resid 102  and name HA  ))
ASSI ( 1614)
   (  segid "BrD " and resid 68   and name HD% )
   (( segid "BrD " and resid 74   and name HB2 ))
     2 900      2.100      2.100 peak  1614 weight  0 10000E+01 volume  0 20510E+03 ppm1      7 790 ppm2      3 010
OR ( 1614)
   (  segid "BrD " and resid 105  and name HD% )
   (( segid "BrD " and resid 109  and name HE2 ))
ASSI ( 1624)
   (  segid "BrD " and resid 34   and name HE% )
   (( segid "BrD " and resid 33   and name HD1 ))
     2 800      2 000      2 000 peak  1624 weight  0 10000E+01 volume  0 23703E+03 ppm1      7 786 ppm2      2 796
OR ( 1624)
   (( segid "BrD " and resid 32   and name HZ3 ))
   (( segid "BrD " and resid 33   and name HD1 ))
OR ( 1624)
   (  segid "BrD " and resid 107  and name HD% )
   (( segid "BrD " and resid 79   and name HB1 ))
OR ( 1624)
   (( segid "BrD " and resid 32   and name HH2 ))
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  (( segid "BrD " and resid 33   and name HD1 ))
ASSI { 1654}
  (  segid "BrD " and resid 34   and name HE% )
  (( segid "BrD " and resid 85   and name HB1 ))
    2.600     1.700     1 700 peak  1654 weight  0 10000E+01 volume  0 36960E+03 ppm1      7 784 ppm2      3 920
OR { 1654}
  (  segid "BrD " and resid 107  and name HD% )
  (( segid "BrD " and resid 106  and name HB1 ))
ASSI { 1664}
  (  segid "BrD " and resid 34   and name HE% )
  (  segid "BrD " and resid 99   and name HB% )
    2 400     1 400     1 400 peak  1664 weight  0 10000E+01 volume  0 66064E+03 ppm1      7 786 ppm2      2 211
OR { 1664}
  (  segid "BrD " and resid 34   and name HE% )
  (( segid "BrD " and resid 33   and name HD2 ))
ASSI { 1674}
  (( segid "BrD " and resid 32   and name HH2 ))
  (( segid "BrD " and resid 33   and name HG1 ))
    3 300     2 700     2 200 peak  1674 weight  0 10000E+01 volume  0 96896E+02 ppm1      7 786 ppm2      0 876
OR { 1674}
  (( segid "BrD " and resid 32   and name HZ3 ))
  (( segid "BrD " and resid 33   and name HG1 ))
OR { 1674}
  (  segid "BrD " and resid 34   and name HE% )
  (( segid "BrD " and resid 33   and name HG1 ))
ASSI { 1684}
  (  segid "BrD " and resid 34   and name HE% )
  (( segid "BrD " and resid 98   and name HA  ))
    3 400     2 900     2 100 peak  1684 weight  0 10000E+01 volume  0 73775E+02 ppm1      7 783 ppm2      4 815
OR { 1684}
  (( segid "BrD " and resid 32   and name HH2 ))
  (( segid "BrD " and resid 94   and name HA  ))
OR { 1684}
  (  segid "BrD " and resid 68   and name HD% )
  (( segid "BrD " and resid 73   and name HA  ))
OR { 1684}
  (  segid "BrD " and resid 107  and name HD% )
  (( segid "BrD " and resid 108  and name HA  ))
OR { 1684}
  (  segid "BrD " and resid 68   and name HD% )
  (( segid "BrD " and resid 60   and name HA  ))
OR { 1684}
  (( segid "BrD " and resid 32   and name HH2 ))
  (( segid "BrD " and resid 98   and name HA  ))
OR { 1684}
  (  segid "BrD " and resid 34   and name HE% )
  (( segid "BrD " and resid 86   and name HA  ))
OR { 1684}
  (  segid "BrD " and resid 107  and name HD% )
  (( segid "BrD " and resid 116  and name HA  ))
OR { 1684}
  (  segid "BrD " and resid 105  and name HD% )
  (( segid "BrD " and resid 108  and name HA  ))
OR { 1684}
  (( segid "BrD " and resid 32   and name HZ3 ))
  (( segid "BrD " and resid 94   and name HA  ))
ASSI { 1704}
  (  segid "BrD " and resid 68   and name HD% )
  (( segid "BrD " and resid 62   and name HD1 ))
    2 700     1 800     1 800 peak  1704 weight  0 10000E+01 volume  0 31213E+03 ppm1      7 787 ppm2      3 153
OR { 1704}
  (  segid "BrD " and resid 105  and name HD% )
  (( segid "BrD " and resid 109  and name HE1 ))
ASSI { 1714}
  (  segid "BrD " and resid 68   and name HD% )
  (( segid "BrD " and resid 62   and name HB1 ))
    2.300     1 300     1 300 peak  1714 weight  0 10000E+01 volume  0 79418E+03 ppm1      7 779 ppm2      2 602
OR { 1714}
  (  segid "BrD " and resid 107  and name HD% )
  (( segid "BrD " and resid 103  and name HG1 ))
OR { 1714}
  (  segid "BrD " and resid 68   and name HD% )
  (( segid "BrD " and resid 62   and name HD2 ))
ASSI { 1734}
  (  segid "BrD " and resid 68   and name HD% )
  (( segid "BrD " and resid 62   and name HG1 ))
    2 900     2 100     2 100 peak  1734 weight  0 10000E+01 volume  0 18466E+03 ppm1      7 781 ppm2      2 324
OR { 1734}
  (  segid "BrD " and resid 34   and name HE% )
  (  segid "BrD " and resid 31   and name HB% )
OR { 1734}
  (  segid "BrD " and resid 107  and name HD% )
  (( segid "BrD " and resid 110  and name HB  ))
OR { 1734}
  (  segid "BrD " and resid 68   and name HD% )
  (( segid "BrD " and resid 73   and name HG  ))
ASSI { 1744}
  (  segid "BrD " and resid 107  and name HD% )
  (( segid "BrD " and resid 110  and name HG12))
    2.300     1 300     1 300 peak  1744 weight  0.10000E+01 volume  0 92480E+03 ppm1      7 781 ppm2      1 641
OR { 1744}
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  (  segid "BrD " and resid 34   and name HE% )
  (  segid "BrD " and resid 25   and name HG2%)
ASSI { 1784}
  (  segid "BrD " and resid 68   and name HD% )
  (( segid "BrD " and resid 62   and name HG1 ))
    2 800     2 000     2 000 peak  1784 weight  0.10000E+01 volume  0 24728E+03 ppm1      7 781 ppm2      2.374
OR { 1784}
  (  segid "BrD " and resid 107  and name HD% )
  (( segid "BrD " and resid 110  and name HB  ))
OR { 1784}
  (  segid "BrD " and resid 68   and name HD% )
  (( segid "BrD " and resid 73   and name HG  ))
ASSI { 1804}
  (  segid "BrD " and resid 68   and name HD% )
  (( segid "BrD " and resid 62   and name HG2 ))
    2.700     1 800     1.800 peak  1804 weight  0 10000E+01 volume  0 30580E+03 ppm1      7 781 ppm2      1 503
OR { 1804}
  (  segid "BrD " and resid 68   and name HD% )
  (  segid "BrD " and resid 73   and name HD2%)
ASSI { 1884}
  (  segid "BrD " and resid 96   and name HD% )
  (( segid "BrD " and resid 92   and name HB1 ))
    2.900     2 100     2.100 peak  1884 weight  0 10000E+01 volume  0 22072E+03 ppm1      7 726 ppm2      2 666
OR { 1884}
  (  segid "BrD " and resid 34   and name HD% )
  (( segid "BrD " and resid 56   and name HB1 ))
ASSI { 1924}
  (  segid "BrD " and resid 96   and name HD% )
  (  segid "BrD " and resid 99   and name HB% )
    2.500     1.600     1 600 peak  1924 weight  0.10000E+01 volume  0 55506E+03 ppm1      7 721 ppm2      2 211
OR { 1924}
  (  segid "BrD " and resid 34   and name HD% )
  (( segid "BrD " and resid 33   and name HD2 ))
ASSI { 1964}
  (  segid "BrD " and resid 96   and name HD% )
  (( segid "BrD " and resid 92   and name HG1 ))
    2.800     2 000     2 000 peak  1964 weight  0 10000E+01 volume  0 22599E+03 ppm1      7 714 ppm2      2 796
OR { 1964}
  (  segid "BrD " and resid 34   and name HD% )
  (( segid "BrD " and resid 33   and name HD1 ))
OR { 1964}
  (  segid "BrD " and resid 34   and name HD% )
  (  segid "BrD " and resid 35   and name HE% )
ASSI { 1974}
  (  segid "BrD " and resid 96   and name HD% )
  (( segid "BrD " and resid 86   and name HB1 ))
    2 300     2 300     2 200 peak  1974 weight  0 10000E+01 volume  0 79213E+03 ppm1      7 717 ppm2      2 321
OR { 1974}
  (  segid "BrD " and resid 34   and name HD% )
  (  segid "BrD " and resid 31   and name HB% )
ASSI { 1994}
  (  segid "BrD " and resid 34   and name HD% )
  (  segid "BrD " and resid 81   and name HG2%)
    2.400     1 400     1.400 peak  1994 weight  0 10000E+01 volume  0 69140E+03 ppm1      7 717 ppm2      0 762
OR { 1994}
  (  segid "BrD " and resid 96   and name HD% )
  (( segid "BrD " and resid 86   and name HG2 ))
ASSI { 2054}
  (  segid "BrD " and resid 34   and name HD% )
  (( segid "BrD " and resid 81   and name HB  ))
    2.900     2 100     2 100 peak  2054 weight  0 10000E+01 volume  0 18901E+03 ppm1      7 709 ppm2      2 033
OR { 2054}
  (  segid "BrD " and resid 34   and name HD% )
  (( segid "BrD " and resid 56   and name HB2 ))
ASSI { 2064}
  (  segid "BrD " and resid 34   and name HD% )
  (( segid "BrD " and resid 33   and name HB1 ))
    2.800     2 000     2 000 peak  2064 weight  0 10000E+01 volume  0 24003E+03 ppm1      7 714 ppm2      1 088
OR { 2064}
  (  segid "BrD " and resid 34   and name HD% )
  (  segid "BrD " and resid 81   and name HG1%)
ASSI { 2134}
  (  segid "BrD " and resid 15   and name HD% )
  (( segid "BrD " and resid 19   and name HE1 ))
    4 000     4 000     1 500 peak  2134 weight  0 10000E+01 volume  0.29314E+02 ppm1      7.692 ppm2      3 512
OR { 2134}
  (  segid "BrD " and resid 96   and name HD% )
  (( segid "BrD " and resid 89   and name HB2 ))
ASSI { 2274}
  (  segid "BrD " and resid 106  and name HE% )
  (  segid "BrD " and resid 59   and name HE% )
    3.400     2 900     2.100 peak  2274 weight  0 10000E+01 volume  0 79128E+02 ppm1      7 640 ppm2      1 820
OR { 2274}
  (  segid "BrD " and resid 106  and name HE% )
  (  segid "BrD " and resid 25   and name HG1%)
ASSI { 2294}
  (  segid "BrD " and resid 106  and name HE% )
  (  segid "BrD " and resid 21   and name HG2%)
    2 600     1.700     1 700 peak  2294 weight  0 10000E+01 volume  0 41702E+03 ppm1      7 643 ppm2      1 593
OR { 2294}
  (  segid "BrD " and resid 106  and name HE% )
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  (( segid "BrD " and resid 116  and name HG12))
ASSI { 2314}
  ( segid "BrD " and resid 106  and name HE% )
  (( segid "BrD " and resid 106  and name HB2 ))
    4 000     4 000     1 500 peak  2314 weight  0 10000E+01 volume  0 29399E+02 ppm1      7 633 ppm2      3 693
OR { 2314}
  ( segid "BrD " and resid 95   and name HE% )
  (( segid "BrD " and resid 89   and name HB1 ))
OR { 2314}
  ( segid "BrD " and resid 88   and name HD% )
  (( segid "BrD " and resid 89   and name HB1 ))
OR { 2314}
  ( segid "BrD " and resid 106  and name HE% )
  (( segid "BrD " and resid 107  and name HB1 ))
ASSI { 2324}
  ( segid "BrD " and resid 106  and name HE% )
  ( segid "BrD " and resid 21   and name HG2%)
    2 600     1 700     1 700 peak  2324 weight  0 10000E+01 volume  0 43383E+03 ppm1      7 616 ppm2      1 576
OR { 2324}
  ( segid "BrD " and resid 88   and name HD% )
  ( segid "BrD " and resid 49   and name HG2%)
OR { 2324}
  ( segid "BrD " and resid 106  and name HE% )
  (( segid "BrD " and resid 116  and name HG12))
ASSI { 2334}
  ( segid "BrD " and resid 95   and name HE% )
  (( segid "BrD " and resid 33   and name HB1 ))
    2 900     2 100     2 100 peak  2334 weight  0 10000E+01 volume  0 19423E+03 ppm1      7 623 ppm2      1 095
OR { 2334}
  ( segid "BrD " and resid 106  and name HE% )
  ( segid "BrD " and resid 18   and name HD1%)
ASSI { 2344}
  ( segid "BrD " and resid 95   and name HE% )
  (( segid "BrD " and resid 32   and name HZ2 ))
    3 300     2 700     2 200 peak  2344 weight  0 10000E+01 volume  0 91993E+02 ppm1      7 615 ppm2      8 004
OR { 2344}
  ( segid "BrD " and resid 106  and name HE% )
  (( segid "BrD " and resid 107  and name HZ  ))
ASSI { 2354}
  ( segid "BrD " and resid 95   and name HE% )
  (( segid "BrD " and resid 95   and name HA  ))
    3 000     2 200     2 200 peak  2354 weight  0 10000E+01 volume  0 18109E+03 ppm1      7 619 ppm2      4 448
OR { 2354}
  ( segid "BrD " and resid 96   and name HE% )
  (( segid "BrD " and resid 96   and name HA  ))
OR { 2354}
  ( segid "BrD " and resid 106  and name HE% )
  (( segid "BrD " and resid 107  and name HA  ))
OR { 2354}
  ( segid "BrD " and resid 106  and name HE% )
  (( segid "BrD " and resid 79   and name HA  ))
ASSI { 2364}
  ( segid "BrD " and resid 95   and name HE% )
  (( segid "BrD " and resid 33   and name HA  ))
    3 200     2 600     2.300 peak  2364 weight  0 10000E+01 volume  0.11374E+03 ppm1      7 617 ppm2      4 366
OR { 2364}
  ( segid "BrD " and resid 106  and name HE% )
  (( segid "BrD " and resid 21   and name HA  ))
ASSI { 2374}
  ( segid "BrD " and resid 88   and name HD% )
  (( segid "BrD " and resid 87   and name HB1 ))
    3 000     2 200     2 200 peak  2374 weight  0 10000E+01 volume  0 17346E+03 ppm1      7 619 ppm2      2 771
OR { 2374}
  ( segid "BrD " and resid 106  and name HE% )
  (( segid "BrD " and resid 79   and name HB1 ))
OR { 2374}
  ( segid "BrD " and resid 95   and name HE% )
  (( segid "BrD " and resid 33   and name HD1 ))
OR { 2374}
  ( segid "BrD " and resid 88   and name HD% )
  (( segid "BrD " and resid 87   and name HG2 ))
ASSI { 2404}
  ( segid "BrD " and resid 106  and name HE% )
  ( segid "BrD " and resid 75   and name HE% )
    2.800     2.000     2 000 peak  2404 weight  0.10000E+01 volume  0.24430E+03 ppm1      7.615 ppm2      2 618
OR { 2404}
  ( segid "BrD " and resid 88   and name HD% )
  (( segid "BrD " and resid 49   and name HB  ))
ASSI { 2424}
  ( segid "BrD " and resid 88   and name HD% )
  ( segid "BrD " and resid 49   and name HG1%)
    2.600     1 700     1 700 peak  2424 weight  0 10000E+01 volume  0 35330E+03 ppm1      7.616 ppm2      1 658
OR { 2424}
  ( segid "BrD " and resid 106  and name HE% )
  (( segid "BrD " and resid 21   and name HG12))
ASSI { 2454}
  ( segid "BrD " and resid 106  and name HE% )
  (( segid "BrD " and resid 17   and name HB  ))
    2 500     1 600     1.600 peak  2454 weight  0 10000E+01 volume  0.48101E+03 ppm1      7 611 ppm2      4.815
OR { 2454}
  ( segid "BrD " and resid 96   and name HE% )
  (( segid "BrD " and resid 86   and name HA  ))
OR { 2454}
  ( segid "BrD " and resid 96   and name HE% )
  (( segid "BrD " and resid 97   and name HA  ))
OR { 2454}
  ( segid "BrD " and resid 88   and name HD% )
  (( segid "BrD " and resid 87   and name HA  ))
OR { 2454}
  ( segid "BrD " and resid 96   and name HE% )
  (( segid "BrD " and resid 92   and name HA  ))
OR { 2454}
  ( segid "BrD " and resid 95   and name HE% )
  (( segid "BrD " and resid 94   and name HA  ))
ASSI { 2524}
  ( segid "BrD " and resid 106  and name HE% )
  (( segid "BrD " and resid 116  and name HG11))
    3 000     2 200     2 200 peak  2524 weight  0 10000E+01 volume  0.18273E+03 ppm1      7 611 ppm2      1 925
OR { 2524}
  ( segid "BrD " and resid 96   and name HE% )
  (( segid "BrD " and resid 86   and name HG1 ))
OR { 2524}
  ( segid "BrD " and resid 96   and name HE% )
  (( segid "BrD " and resid 86   and name HD1 ))
ASSI { 2544}
  ( segid "BrD " and resid 106  and name HD% )
  (( segid "BrD " and resid 107  and name HA  ))
    3.100     2 400     2.400 peak  2544 weight  0 10000E+01 volume  0 12798E+03 ppm1      7 538 ppm2      4 390
OR { 2544}
  ( segid "BrD " and resid 106  and name HD% )
  (( segid "BrD " and resid 79   and name HA  ))
OR { 2544}
  ( segid "BrD " and resid 74   and name HE% )
  (( segid "BrD " and resid 74   and name HA  ))
ASSI { 2604}
  ( segid "BrD " and resid 74   and name HE% )
  (( segid "BrD " and resid 59   and name HB1 ))
    2 500     1.600     1 600 peak  2604 weight  0 10000E+01 volume  0 55016E+03 ppm1      7.534 ppm2      2.695
OR { 2604}
  ( segid "BrD " and resid 74   and name HE% )
  (( segid "BrD " and resid 22   and name HB1 ))
ASSI { 2624}
  ( segid "BrD " and resid 106  and name HD% )
  (( segid "BrD " and resid 109  and name HB2 ))
    3.000     2 200     2 200 peak  2624 weight  0.10000E+01 volume  0 15519E+03 ppm1      7 534 ppm2      2 146
OR { 2624}
  ( segid "BrD " and resid 74   and name HE% )
  (( segid "BrD " and resid 18   and name HB1 ))
ASSI { 2644}
  ( segid "BrD " and resid 74   and name HE% )
  (( segid "BrD " and resid 63   and name HB2 ))
    2 300     1 300     1 300 peak  2644 weight  0.10000E+01 volume  0.82012E+03 ppm1      7 531 ppm2      2 521
OR { 2644}
  ( segid "BrD " and resid 106  and name HD% )
  (( segid "BrD " and resid 21   and name HB  ))
ASSI { 2664}
  ( segid "BrD " and resid 106  and name HD% )
  ( segid "BrD " and resid 102  and name HD2%)
    2 800     2 000     2 000 peak  2664 weight  0 10000E+01 volume  0 24374E+03 ppm1      7.530 ppm2      1 331
OR { 2664}
  ( segid "BrD " and resid 74   and name HE% )
  (( segid "BrD " and resid 78   and name HB1 ))
ASSI { 2784}
  ( segid "BrD " and resid 74   and name HE% )
  (( segid "BrD " and resid 68   and name HB2 ))
    2.900     2 100     2 100 peak  2784 weight  0.10000E+01 volume  0 21978E+03 ppm1      7 530 ppm2      3 559
OR { 2784}
  ( segid "BrD " and resid 74   and name HE% )
  (( segid "BrD " and resid 74   and name HB1 ))
OR { 2784}
  ( segid "BrD " and resid 95   and name HD% )
  (( segid "BrD " and resid 88   and name HB1 ))
ASSI { 2804}
  ( segid "BrD " and resid 95   and name HD% )
  (( segid "BrD " and resid 32   and name HH2 ))
    2.800     2 000     2 000 peak  2804 weight  0.10000E+01 volume  0.23332E+03 ppm1      7 520 ppm2      7 793
OR { 2804}
  ( segid "BrD " and resid 106  and name HD% )
  ( segid "BrD " and resid 107  and name HD% )
ASSI { 2814}
  ( segid "BrD " and resid 106  and name HD% )
  (( segid "BrD " and resid 78   and name HB2 ))
    3.000     2.200     2.200 peak  2814 weight  0 10000E+01 volume  0.16253E+03 ppm1      7 520 ppm2      1.080
OR { 2814}
  ( segid "BrD " and resid 74   and name HE% )
  ( segid "BrD " and resid 18   and name HD1%)
OR { 2814}
  ( segid "BrD " and resid 95   and name HD% )
  (( segid "BrD " and resid 33   and name HB1 ))
ASSI { 2914}
  ( segid "BrD " and resid 15   and name HE% )
  (( segid "BrD " and resid 19   and name HE1 ))
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    2.900     2.100     2.100 peak  2914 weight  0.10000E+01 volume  0.20135E+03 ppm1      7.488 ppm2      3.545
OR { 2914}
  ( segid "BrD " and resid 95   and name HD% )
  (( segid "BrD " and resid 86   and name HB1 ))
ASSI { 3164}
  ( segid "BrD " and resid 82   and name HD% )
  (( segid "BrD " and resid 103  and name HB1 ))
    2.700     1.800     1.800 peak  3164 weight  0.10000E+01 volume  0.29307E+03 ppm1      7.270 ppm2      2.309
OR { 3164}
  ( segid "BrD " and resid 47   and name HE% )
  (( segid "BrD " and resid 37   and name HB2 ))
ASSI { 3284}
  ( segid "BrD " and resid 82   and name HD% )
  ( segid "BrD " and resid 34   and name HE% )
    2.800     2.000     2.000 peak  3284 weight  0.10000E+01 volume  0.24491E+03 ppm1      7.263 ppm2      7.800
OR { 3284}
  ( segid "BrD " and resid 82   and name HD% )
  ( segid "BrD " and resid 107  and name HD% )
ASSI { 3324}
  ( segid "BrD " and resid 82   and name HE% )
  (( segid "BrD " and resid 79   and name HA ))
    2.900     2.100     2.100 peak  3324 weight  0.10000E+01 volume  0.20070E+03 ppm1      7.074 ppm2      4.440
OR { 3324}
  ( segid "BrD " and resid 82   and name HE% )
  (( segid "BrD " and resid 107  and name HA ))
ASSI { 3394}
  ( segid "BrD " and resid 82   and name HE% )
  (( segid "BrD " and resid 81   and name HB ))
    2.600     1.700     1.700 peak  3394 weight  0.10000E+01 volume  0.37424E+03 ppm1      7.069 ppm2      2.032
OR { 3394}
  ( segid "BrD " and resid 82   and name HE% )
  (( segid "BrD " and resid 102  and name HB1 ))
ASSI { 3414}
  ( segid "BrD " and resid 82   and name HE% )
  ( segid "BrD " and resid 25   and name HG2% )
    3.400     2.900     2.100 peak  3414 weight  0.10000E+01 volume  0.73603E+02 ppm1      7.067 ppm2      1.641
OR { 3414}
  ( segid "BrD " and resid 82   and name HE% )
  (( segid "BrD " and resid 110  and name HG12 ))
ASSI { 3474}
  (( segid "BrD " and resid 82   and name HZ  ))
  (( segid "BrD " and resid 102  and name HG  ))
    2.800     2.000     2.000 peak  3474 weight  0.10000E+01 volume  0.23859E+03 ppm1      7.025 ppm2      2.163
OR { 3474}
  ( segid "BrD " and resid 74   and name HD% )
  (( segid "BrD " and resid 18   and name HB1 ))
ASSI { 3484}
  ( segid "BrD " and resid 74   and name HD% )
  ( segid "BrD " and resid 78   and name HD1% )
    2.900     2.100     2.100 peak  3484 weight  0.10000E+01 volume  0.18792E+03 ppm1      7.023 ppm2      0.780
OR { 3484}
  (( segid "BrD " and resid 82   and name HZ  ))
  ( segid "BrD " and resid 78   and name HD1% )
ASSI { 3494}
  ( segid "BrD " and resid 74   and name HD% )
  (( segid "BrD " and resid 68   and name HB1 ))
    2.900     2.100     2.100 peak  3494 weight  0.10000E+01 volume  0.19853E+03 ppm1      7.022 ppm2      3.708
OR { 3494}
  (( segid "BrD " and resid 82   and name HZ  ))
  (( segid "BrD " and resid 106  and name HB2 ))
ASSI { 3504}
  (( segid "BrD " and resid 82   and name HZ  ))
  (( segid "BrD " and resid 81   and name HB  ))
    3.100     2.400     2.400 peak  3504 weight  0.10000E+01 volume  0.12383E+03 ppm1      7.023 ppm2      2.034
OR { 3504}
  ( segid "BrD " and resid 74   and name HD% )
  (( segid "BrD " and resid 14   and name HG  ))
ASSI { 3544}
  ( segid "BrD " and resid 74   and name HD% )
  (( segid "BrD " and resid 18   and name HG  ))
    3.400     2.900     2.100 peak  3544 weight  0.10000E+01 volume  0.82384E+02 ppm1      7.005 ppm2      2.307
OR { 3544}
  (( segid "BrD " and resid 82   and name HZ  ))
  (( segid "BrD " and resid 103  and name HB1 ))
OR { 3544}
  ( segid "BrD " and resid 74   and name HD% )
  (( segid "BrD " and resid 21   and name HG11 ))
OR { 3544}
  ( segid "BrD " and resid 74   and name HD% )
  (( segid "BrD " and resid 62   and name HG1 ))
OR { 3544}
  ( segid "BrD " and resid 74   and name HD% )
  (( segid "BrD " and resid 73   and name HG  ))
OR { 3544}
  (( segid "BrD " and resid 82   and name HZ  ))
  (( segid "BrD " and resid 21   and name HG11 ))
ASSI { 3554}
  ( segid "BrD " and resid 74   and name HD% )
  ( segid "BrD " and resid 63   and name HD1% )
    2.500     1.600     1.600 peak  3554 weight  0.10000E+01 volume  0.51806E+03 ppm1      7.009 ppm2      1.641
OR { 3554}
  ( segid "BrD " and resid 74   and name HD% )
  ( segid "BrD " and resid 22   and name HD1% )
ASSI { 3564}
  ( segid "BrD " and resid 74   and name HD% )
  ( segid "BrD " and resid 68   and name HE% )
    3.100     2.400     2.400 peak  3564 weight  0.10000E+01 volume  0.13987E+03 ppm1      7.005 ppm2      7.889
OR { 3564}
  (( segid "BrD " and resid 82   and name HZ  ))
  ( segid "BrD " and resid 107  and name HE% )
ASSI { 3584}
  ( segid "BrD " and resid 74   and name HD% )
  ( segid "BrD " and resid 106  and name HE% )
    3.000     2.200     2.200 peak  3584 weight  0.10000E+01 volume  0.17632E+03 ppm1      7.005 ppm2      7.647
OR { 3584}
  (( segid "BrD " and resid 82   and name HZ  ))
  ( segid "BrD " and resid 106  and name HE% )
ASSI { 3604}
  ( segid "BrD " and resid 74   and name HD% )
  (( segid "BrD " and resid 71   and name HA  ))
    3.300     2.700     2.200 peak  3604 weight  0.10000E+01 volume  0.95504E+02 ppm1      7.005 ppm2      4.636
OR { 3604}
  ( segid "BrD " and resid 74   and name HD% )
  (( segid "BrD " and resid 15   and name HA  ))
OR { 3604}
  ( segid "BrD " and resid 74   and name HD% )
  (( segid "BrD " and resid 76   and name HA  ))
OR { 3604}
  ( segid "BrD " and resid 74   and name HD% )
  (( segid "BrD " and resid 56   and name HA  ))
OR { 3604}
  ( segid "BrD " and resid 74   and name HD% )
  (( segid "BrD " and resid 72   and name HA  ))
OR { 3604}
  ( segid "BrD " and resid 74   and name HD% )
  (( segid "BrD " and resid 14   and name HA  ))
OR { 3604}
  ( segid "BrD " and resid 74   and name HD% )
  (( segid "BrD " and resid 67   and name HA  ))
OR { 3604}
  ( segid "BrD " and resid 74   and name HD% )
  (( segid "BrD " and resid 60   and name HB2 ))
OR { 3604}
  (( segid "BrD " and resid 82   and name HZ  ))
  (( segid "BrD " and resid 104  and name HA  ))
ASSI { 3634}
  ( segid "BrD " and resid 74   and name HD% )
  (( segid "BrD " and resid 75   and name HG2 ))
    3.100     2.400     2.400 peak  3634 weight  0.10000E+01 volume  0.12756E+03 ppm1      7.004 ppm2      3.221
OR { 3634}
  ( segid "BrD " and resid 74   and name HD% )
  (( segid "BrD " and resid 59   and name HG1 ))
OR { 3634}
  ( segid "BrD " and resid 74   and name HD% )
  (( segid "BrD " and resid 59   and name HG2 ))
ASSI { 3664}
  ( segid "BrD " and resid 74   and name HD% )
  (( segid "BrD " and resid 63   and name HB2 ))
    3.600     3.200     1.900 peak  3664 weight  0.10000E+01 volume  0.57581E+02 ppm1      7.005 ppm2      2.520
OR { 3664}
  (( segid "BrD " and resid 82   and name HZ  ))
  (( segid "BrD " and resid 21   and name HB  ))
ASSI { 3674}
  (( segid "BrD " and resid 82   and name HZ  ))
  (( segid "BrD " and resid 21   and name HB  ))
    3.700     3.400     1.800 peak  3674 weight  0.10000E+01 volume  0.46728E+02 ppm1      7.004 ppm2      2.494
OR { 3674}
  ( segid "BrD " and resid 74   and name HD% )
  (( segid "BrD " and resid 59   and name HB2 ))
OR { 3674}
  ( segid "BrD " and resid 74   and name HD% )
  (( segid "BrD " and resid 73   and name HB2 ))
ASSI { 3694}
  ( segid "BrD " and resid 74   and name HD% )
  ( segid "BrD " and resid 63   and name HD2% )
    3.500     3.100     2.000 peak  3694 weight  0.10000E+01 volume  0.62447E+02 ppm1      7.005 ppm2      1.496
OR { 3694}
  ( segid "BrD " and resid 74   and name HD% )
  ( segid "BrD " and resid 73   and name HD2% )
ASSI { 3854}
  ( segid "BrD " and resid 46   and name HE% )
  (( segid "BrD " and resid 50   and name HG12 ))
    2.700     1.800     1.800 peak  3854 weight  0.10000E+01 volume  0.29261E+03 ppm1      6.687 ppm2      0.795
OR { 3854}
  ( segid "BrD " and resid 46   and name HE% )
  ( segid "BrD " and resid 38   and name HG2% )
ASSI { 3954}
  ( segid "BrD " and resid 46   and name HD% )
  (( segid "BrD " and resid 50   and name HG12 ))
    3.200     2.600     2.300 peak  3954 weight  0.10000E+01 volume  0.11437E+03 ppm1      5.740 ppm2      0.796
OR { 3954}
  ( segid "BrD " and resid 46   and name HD% )
```

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   (  segid "BrD " and resid 38   and name HG2%)
ASSI { 4144}
   (  segid "BrD " and resid 74   and name HD% )
   (( segid "BrD " and resid 78   and name HG  ))
     3 400      2 900      2 100 peak  4144 weight  0.10000E+01 volume  0 77150E+02 ppm1      7.005 ppm2      1 249
OR { 4144}
   (( segid "BrD " and resid 82   and name HZ  ))
   (( segid "BrD " and resid 78   and name HG  ))
ASSI { 4154}
   (  segid "BrD " and resid 74   and name HE% )
   (  segid "BrD " and resid 22   and name HD1%)
     2.400      1 400      1 400 peak  4154 weight  0 10000E+01 volume  0 70341E+03 ppm1      7 534 ppm2      1 676
OR { 4154}
   (  segid "BrD " and resid 106  and name HD% )
   (( segid "BrD " and resid 21   and name HG12))
ASSI { 4174}
   (  segid "BrD " and resid 96   and name HD% )
   (( segid "BrD " and resid 100  and name HA  ))
     3 100      2 400      2 400 peak  4174 weight  0 10000E+01 volume  0 13533E+03 ppm1      7 689 ppm2      4 927
OR { 4174}
   (  segid "BrD " and resid 34   and name HD% )
   (( segid "BrD " and resid 35   and name HA  ))
OR { 4174}
   (  segid "BrD " and resid 15   and name HD% )
   (( segid "BrD " and resid 64   and name HA  ))
OR { 4174}
   (  segid "BrD " and resid 15   and name HD% )
   (( segid "BrD " and resid 11   and name HA  ))
OR { 4174}
   (  segid "BrD " and resid 34   and name HD% )
   (( segid "BrD " and resid 32   and name HA  ))
ASSI { 4224}
   (  segid "BrD " and resid 88   and name HD% )
   (( segid "BrD " and resid 50   and name HG12))
     3 100      2 400      2 400 peak  4224 weight  0 10000E+01 volume  0 12837E+03 ppm1      7 615 ppm2      0 845
OR { 4224}
   (  segid "BrD " and resid 95   and name HE% )
   (( segid "BrD " and resid 33   and name HG1 ))
ASSI { 4234}
   (  segid "BrD " and resid 96   and name HE% )
   (  segid "BrD " and resid 99   and name HB% )
     3 300      2 700      2 200 peak  4234 weight  0.10000E+01 volume  0 94963E+02 ppm1      7 611 ppm2      2 178
OR { 4234}
   (  segid "BrD " and resid 106  and name HE% )
   (( segid "BrD " and resid 18   and name HB1 ))
OR { 4234}
   (  segid "BrD " and resid 106  and name HE% )
   (( segid "BrD " and resid 109  and name HB2 ))
OR { 4234}
   (  segid "BrD " and resid 106  and name HE% )
   (( segid "BrD " and resid 115  and name HB1 ))
OR { 4234}
   (  segid "BrD " and resid 106  and name HE% )
   (( segid "BrD " and resid 115  and name HG  ))
ASSI { 4244}
   (  segid "BrD " and resid 106  and name HE% )
   (  segid "BrD " and resid 78   and name HD1%)
     3 100      2 400      2 400 peak  4244 weight  0 10000E+01 volume  0 14012E+03 ppm1      7 616 ppm2      0.763
OR { 4244}
   (  segid "BrD " and resid 96   and name HE% )
   (( segid "BrD " and resid 86   and name HG2 ))
ASSI { 4284}
   (  segid "BrD " and resid 74   and name HE% )
   (( segid "BrD " and resid 74   and name HB2 ))
     3 000      2.200      2 200 peak  4284 weight  0.10000E+01 volume  0 18031E+03 ppm1      7 534 ppm2      3 010
OR { 4284}
   (  segid "BrD " and resid 106  and name HD% )
   (( segid "BrD " and resid 109  and name HE2 ))
ASSI { 4344}
   (( segid "BrD " and resid 34   and name HZ  ))
   (( segid "BrD " and resid 28   and name HD2 ))
     3 100      2 400      2.400 peak  4344 weight  0 10000E+01 volume  0 12962E+03 ppm1      7 904 ppm2      5 555
OR { 4344}
   (  segid "BrD " and resid 68   and name HE% )
   (( segid "BrD " and resid 54   and name HA  ))
ASSI { 4354}
   (  segid "BrD " and resid 106  and name HD% )
   (( segid "BrD " and resid 78   and name HB2 ))
     2 900      2 100      2.100 peak  4354 weight  0.10000E+01 volume  0.19182E+03 ppm1      7.539 ppm2      1 089
OR { 4354}
   (  segid "BrD " and resid 74   and name HE% )
   (  segid "BrD " and resid 18   and name HD1%)
```

Table 4

Hydrogen Bonding Restraints

```
!Helix Z
assign (residue 19 and name HN  ) (residue 15  and name O )     1.80  0.0  0.40
assign (residue 19 and name N   ) (residue 15  and name O )     2.80  0.30 0.40

assign (residue 22 and name HN  ) (residue 18  and name O )     1.80  0.0  0.40
assign (residue 22 and name N   ) (residue 18  and name O )     2.80  0.30 0.40

assign (residue 23 and name HN  ) (residue 19  and name O )     1.80  0.0  0.40
assign (residue 23 and name N   ) (residue 19  and name O )     2.80  0.30 0.40

assign (residue 24 and name HN  ) (residue 20  and name O )     1.80  0.0  0.40
assign (residue 24 and name N   ) (residue 20  and name O )     2.80  0.30 0.40

assign (residue 25 and name HN  ) (residue 21  and name O )     1.80  0.0  0.40
assign (residue 25 and name N   ) (residue 21  and name O )     2.80  0.30 0.40


!Helix B
assign (residue 75 and name HN  ) (residue 71  and name O )     1.80  0.0  0.40
assign (residue 75 and name N   ) (residue 71  and name O )     2.80  0.30 0.40

!assign (residue 77 and name HN  ) (residue 73  and name O )     1.80  0.0  0.40
!assign (residue 77 and name N   ) (residue 73  and name O )     2.80  0.30 0.40

assign (residue 78 and name HN  ) (residue 74  and name O )     1.80  0.0  0.40
assign (residue 78 and name N   ) (residue 74  and name O )     2.80  0.30 0.40

assign (residue 79 and name HN  ) (residue 75  and name O )     1.80  0.0  0.40
assign (residue 79 and name N   ) (residue 75  and name O )     2.80  0.30 0.40

!assign (residue 80 and name HN  ) (residue 76  and name O )     1.80  0.0  0.40
!assign (residue 80 and name N   ) (residue 76  and name O )     2.80  0.30 0.40

assign (residue 81 and name HN  ) (residue 77  and name O )     1.80  0.0  0.40
assign (residue 81 and name N   ) (residue 77  and name O )     2.80  0.30 0.40

assign (residue 82 and name HN  ) (residue 78  and name O )     1.80  0.0  0.40
assign (residue 82 and name N   ) (residue 78  and name O )     2.80  0.30 0.40

!Helix C
assign (residue 102 and name HN  ) (residue 98 and name O )     1.80  0.0  0.40
assign (residue 102 and name N   ) (residue 98 and name O )     2.80  0.30 0.40

assign (residue 103 and name HN  ) (residue 99 and name O )     1.80  0.0  0.40
assign (residue 103 and name N   ) (residue 99 and name O )     2.80  0.30 0.40

assign (residue 104 and name HN  ) (residue 100 and name O )     1.80  0.0  0.40
assign (residue 104 and name N   ) (residue 100 and name O )     2.80  0.30 0.40

assign (residue 105 and name HN  ) (residue 101 and name O )     1.80  0.0  0.40
assign (residue 105 and name N   ) (residue 101 and name O )     2.80  0.30 0.40
```

Table 5

Atomic Structure Coordinates of the Free Form of the P/CAF Bromodomain

```
REMARK FILENAME="/bloch2/chris/BROMO_XPLOR_ARIA32/structures/it8/brd_187.pdb"
REMARK initial random number seed 1.342876E+11
REMARK ===============================================================
REMARK              overall,bonds,angles,improper,vdw,noe,cdih
REMARK energies: 157.923, 9.30626, 73.1523, 0, 23.1819, 36.4277, 0.228429
REMARK ===============================================================
REMARK              bonds,angles,impropers,noe,cdih
REMARK rms-dev   2.164156E-03,0.365411,50.3111,1.418985E-02,0.263503
REMARK ===============================================================
REMARK                   noe,  cdih
REMARK violations : 2, 0
REMARK ===============================================================
REMARK DATE 29-Nov-98  06 51 33       created by user
ATOM      1  CA  GLY     1      27.208  16.825  -6.349  1.00  0.00
ATOM      2  HA1 GLY     1      26.763  16.827  -5.365  1.00  0.00
ATOM      3  HA2 GLY     1      28.041  17.514  -6.357  1.00  0.00
ATOM      4  C   GLY     1      27.723  15.432  -6.650  1.00  0.00
ATOM      5  O   GLY     1      28.656  15.263  -7.435  1.00  0.00
ATOM      6  N   GLY     1      26.194  17.285  -7.337  1.00  0.00
ATOM      7  HT1 GLY     1      26.586  18.049  -7.923  1.00  0.00
ATOM      8  HT2 GLY     1      25.350  17.641  -6.843  1.00  0.00
ATOM      9  HT3 GLY     1      25.914  16.498  -7.955  1.00  0.00
ATOM     10  N   SER     2      27.113  14.431  -6.024  1.00  0.00
ATOM     11  HN  SER     2      26.376  14.629  -5.409  1.00  0.00
ATOM     12  CA  SER     2      27.516  13.044  -6.226  1.00  0.00
ATOM     13  HA  SER     2      28.481  13.047  -6.712  1.00  0.00
ATOM     14  CB  SER     2      27.638  12.329  -4.878  1.00  0.00
ATOM     15  HB1 SER     2      26.904  12.729  -4.193  1.00  0.00
ATOM     16  HB2 SER     2      27.462  11.273  -5.017  1.00  0.00
ATOM     17  OG  SER     2      28.927  12.508  -4.319  1.00  0.00
ATOM     18  HG  SER     2      29.571  12.014  -4.832  1.00  0.00
ATOM     19  C   SER     2      26.519  12.308  -7.114  1.00  0.00
ATOM     20  O   SER     2      25.320  12.288  -6.835  1.00  0.00
ATOM     21  N   HIS     3      27.022  11.698  -8.183  1.00  0.00
ATOM     22  HN  HIS     3      27.986  11.747  -8.353  1.00  0.00
ATOM     23  CA  HIS     3      26.173  10.955  -9.106  1.00  0.00
ATOM     24  HA  HIS     3      25.157  11.295  -8.967  1.00  0.00
ATOM     25  CB  HIS     3      26.594  11.222 -10.553  1.00  0.00
ATOM     26  HB1 HIS     3      26.616  12.288 -10.723  1.00  0.00
ATOM     27  HB2 HIS     3      27.581  10.814 -10.714  1.00  0.00
ATOM     28  CG  HIS     3      25.671  10.612 -11.561  1.00  0.00
ATOM     29  ND1 HIS     3      25.985  10.494 -12.900  1.00  0.00
ATOM     30  HD1 HIS     3      26.820  10.790 -13.320  1.00  0.00
ATOM     31  CD2 HIS     3      24.433  10.080 -11.420  1.00  0.00
ATOM     32  HD2 HIS     3      23.870  10.003 -10.501  1.00  0.00
ATOM     33  CE1 HIS     3      24.981   9.918 -13.537  1.00  0.00
ATOM     34  HE1 HIS     3      24.945   9.698 -14.594  1.00  0.00
ATOM     35  NE2 HIS     3      24.028   9.658 -12.662  1.00  0.00
ATOM     36  HE2 HIS     3      23.171   9.230 -12.868  1.00  0.00
ATOM     37  C   HIS     3      26.233   9.459  -8.817  1.00  0.00
ATOM     38  O   HIS     3      26.214   8.638  -9.734  1.00  0.00
ATOM     39  N   MET     4      26.305   9.111  -7.536  1.00  0.00
ATOM     40  HN  MET     4      26.314   9.811  -6.850  1.00  0.00
ATOM     41  CA  MET     4      26.364   7.713  -7.128  1.00  0.00
ATOM     42  HA  MET     4      26.164   7.105  -7.998  1.00  0.00
ATOM     43  CB  MET     4      27.755   7.374  -6.591  1.00  0.00
ATOM     44  HB1 MET     4      28.456   8.117  -6.944  1.00  0.00
ATOM     45  HB2 MET     4      27.730   7.400  -5.512  1.00  0.00
ATOM     46  CG  MET     4      28.254   6.005  -7.024  1.00  0.00
ATOM     47  HG1 MET     4      27.433   5.306  -6.972  1.00  0.00
ATOM     48  HG2 MET     4      28.606   6.071  -8.043  1.00  0.00
ATOM     49  SD  MET     4      29.597   5.394  -5.988  1.00  0.00
ATOM     50  CE  MET     4      28.922   3.825  -5.449  1.00  0.00
ATOM     51  HE1 MET     4      29.243   3.623  -4.438  1.00  0.00
ATOM     52  HE2 MET     4      29.273   3.039  -6.102  1.00  0.00
ATOM     53  HE3 MET     4      27.843   3.866  -5.483  1.00  0.00
ATOM     54  C   MET     4      25.310   7.413  -6.067  1.00  0.00
ATOM     55  O   MET     4      25.333   7.983  -4.977  1.00  0.00
ATOM     56  N   SER     5      24.386   6.517  -6.398  1.00  0.00
ATOM     57  HN  SER     5      24.422   6.098  -7.283  1.00  0.00
ATOM     58  CA  SER     5      23.321   6.141  -5.476  1.00  0.00
ATOM     59  HA  SER     5      23.780   5.750  -4.580  1.00  0.00
ATOM     60  CB  SER     5      22.479   7.366  -5.111  1.00  0.00
ATOM     61  HB1 SER     5      22.188   7.882  -6.014  1.00  0.00
ATOM     62  HB2 SER     5      23.062   8.029  -4.490  1.00  0.00
ATOM     63  OG  SER     5      21.309   6.990  -4.405  1.00  0.00
ATOM     64  HG  SER     5      21.060   7.693  -3.800  1.00  0.00
ATOM     65  C   SER     5      22.431   5.062  -6.084  1.00  0.00
ATOM     66  O   SER     5      21.471   5.362  -6.794  1.00  0.00
ATOM     67  N   LYS     6      22.756   3.805  -5.800  1.00  0.00
ATOM     68  HN  LYS     6      23.532   3.630  -5.228  1.00  0.00
ATOM     69  CA  LYS     6      21.987   2.680  -6.319  1.00  0.00
ATOM     70  HA  LYS     6      21.642   2.942  -7.308  1.00  0.00
ATOM     71  CB  LYS     6      22.869   1.433  -6.409  1.00  0.00
ATOM     72  HB1 LYS     6      22.266   0.563  -6.192  1.00  0.00
ATOM     73  HB2 LYS     6      23.655   1.508  -5.673  1.00  0.00
ATOM     74  CG  LYS     6      23.510   1.238  -7.773  1.00  0.00
ATOM     75  HG1 LYS     6      24.045   2.138  -8.041  1.00  0.00
ATOM     76  HG2 LYS     6      24.201   0.409  -7.721  1.00  0.00
ATOM     77  CD  LYS     6      22.469   0.947  -8.842  1.00  0.00
ATOM     78  HD1 LYS     6      21.794   1.787  -8.911  1.00  0.00
ATOM     79  HD2 LYS     6      22.970   0.804  -9.788  1.00  0.00
ATOM     80  CE  LYS     6      21.669  -0.304  -8.514  1.00  0.00
ATOM     81  HE1 LYS     6      21.107  -0.129  -7.608  1.00  0.00
ATOM     82  HE2 LYS     6      20.987  -0.503  -9.327  1.00  0.00
ATOM     83  NZ  LYS     6      22.548  -1.489  -8.317  1.00  0.00
ATOM     84  HZ1 LYS     6      23.320  -1.481  -9.014  1.00  0.00
ATOM     85  HZ2 LYS     6      21.999  -2.365  -8.435  1.00  0.00
ATOM     86  HZ3 LYS     6      22.958  -1.476  -7.362  1.00  0.00
ATOM     87  C   LYS     6      20.776   2.397  -5.436  1.00  0.00
ATOM     88  O   LYS     6      20.863   1.638  -4.471  1.00  0.00
ATOM     89  N   GLU     7      19.646   3.011  -5.773  1.00  0.00
ATOM     90  HN  GLU     7      19.637   3.606  -6.552  1.00  0.00
ATOM     91  CA  GLU     7      18.420   2.825  -5.005  1.00  0.00
ATOM     92  HA  GLU     7      18.531   1.926  -4.418  1.00  0.00
ATOM     93  CB  GLU     7      18.200   4.011  -4.064  1.00  0.00
ATOM     94  HB1 GLU     7      18.505   4.916  -4.567  1.00  0.00
ATOM     95  HB2 GLU     7      17.148   4.078  -3.828  1.00  0.00
ATOM     96  CG  GLU     7      18.975   3.904  -2.761  1.00  0.00
ATOM     97  HG1 GLU     7      19.746   3.156  -2.876  1.00  0.00
ATOM     98  HG2 GLU     7      19.430   4.860  -2.548  1.00  0.00
ATOM     99  CD  GLU     7      18.095   3.515  -1.589  1.00  0.00
ATOM    100  OE1 GLU     7      17.118   4.243  -1.312  1.00  0.00
ATOM    101  OE2 GLU     7      18.383   2.483  -0.947  1.00  0.00
ATOM    102  C   GLU     7      17.215   2.662  -5.928  1.00  0.00
ATOM    103  O   GLU     7      16.278   3.461  -5.886  1.00  0.00
ATOM    104  N   PRO     8      17.218   1.617  -6.772  1.00  0.00
ATOM    105  CA  PRO     8      16.120   1.352  -7.702  1.00  0.00
ATOM    106  HA  PRO     8      15.785   2.256  -8.189  1.00  0.00
ATOM    107  CB  PRO     8      16.760   0.419  -8.727  1.00  0.00
ATOM    108  HB1 PRO     8      17.200   1.002  -9.523  1.00  0.00
ATOM    109  HB2 PRO     8      16.011  -0.245  -9.130  1.00  0.00
ATOM    110  CG  PRO     8      17.796  -0.327  -7.958  1.00  0.00
ATOM    111  HG1 PRO     8      17.357  -1.205  -7.508  1.00  0.00
ATOM    112  HG2 PRO     8      18.607  -0.608  -8.614  1.00  0.00
ATOM    113  CD  PRO     8      18.294   0.613  -6.889  1.00  0.00
ATOM    114  HD1 PRO     8      18.429   0.085  -5.956  1.00  0.00
ATOM    115  HD2 PRO     8      19.220   1.076  -7.197  1.00  0.00
ATOM    116  C   PRO     8      14.938   0.669  -7.021  1.00  0.00
ATOM    117  O   PRO     8      13.782   0.924  -7.360  1.00  0.00
ATOM    118  N   ARG     9      15.236  -0.196  -6.057  1.00  0.00
ATOM    119  HN  ARG     9      16.176  -0.357  -5.833  1.00  0.00
ATOM    120  CA  ARG     9      14.199  -0.917  -5.328  1.00  0.00
ATOM    121  HA  ARG     9      13.522  -0.189  -4.906  1.00  0.00
ATOM    122  CB  ARG     9      13.421  -1.830  -6.279  1.00  0.00
ATOM    123  HB1 ARG     9      12.812  -2.504  -5.695  1.00  0.00
ATOM    124  HB2 ARG     9      12.778  -1.222  -6.898  1.00  0.00
ATOM    125  CG  ARG     9      14.313  -2.661  -7.188  1.00  0.00
ATOM    126  HG1 ARG     9      14.295  -2.236  -8.181  1.00  0.00
ATOM    127  HG2 ARG     9      15.322  -2.640  -6.803  1.00  0.00
ATOM    128  CD  ARG     9      13.843  -4.106  -7.262  1.00  0.00
ATOM    129  HD1 ARG     9      13.831  -4.518  -6.264  1.00  0.00
ATOM    130  HD2 ARG     9      12.844  -4.125  -7.671  1.00  0.00
ATOM    131  NE  ARG     9      14.714  -4.926  -8.102  1.00  0.00
ATOM    132  HE  ARG     9      15.302  -4.464  -8.735  1.00  0.00
ATOM    133  CZ  ARG     9      14.745  -6.255  -8.053  1.00  0.00
ATOM    134  NH1 ARG     9      13.960  -6.908  -7.208  1.00  0.00
ATOM    135 HH11 ARG     9      13.342  -6.401  -6.606  1.00  0.00
ATOM    136 HH12 ARG     9      13.985  -7.907  -7.172  1.00  0.00
ATOM    137  NH2 ARG     9      15.563  -6.932  -8.850  1.00  0.00
ATOM    138 HH21 ARG     9      16.157  -6.444  -9.489  1.00  0.00
ATOM    139 HH22 ARG     9      15.585  -7.931  -8.810  1.00  0.00
ATOM    140  C   ARG     9      14.800  -1.744  -4.196  1.00  0.00
ATOM    141  O   ARG     9      14.421  -2.897  -3.991  1.00  0.00
ATOM    142  N   ASP    10      15.732  -1.144  -3.458  1.00  0.00
ATOM    143  HN  ASP    10      15.988  -0.223  -3.673  1.00  0.00
ATOM    144  CA  ASP    10      16.393  -1.824  -2.345  1.00  0.00
ATOM    145  HA  ASP    10      17.087  -2.540  -2.760  1.00  0.00
ATOM    146  CB  ASP    10      17.169  -0.813  -1.497  1.00  0.00
ATOM    147  HB1 ASP    10      17.594  -0.061  -2.146  1.00  0.00
ATOM    148  HB2 ASP    10      16.490  -0.341  -0.802  1.00  0.00
ATOM    149  CG  ASP    10      18.292  -1.457  -0.708  1.00  0.00
ATOM    150  OD1 ASP    10      18.771  -2.532  -1.126  1.00  0.00
ATOM    151  OD2 ASP    10      18.692  -0.886   0.328  1.00  0.00
ATOM    152  C   ASP    10      15.383  -2.565  -1.468  1.00  0.00
ATOM    153  O   ASP    10      14.728  -1.961  -0.619  1.00  0.00
ATOM    154  N   PRO    11      15.249  -3.889  -1.658  1.00  0.00
ATOM    155  CA  PRO    11      14.309  -4.709  -0.887  1.00  0.00
ATOM    156  HA  PRO    11      13.311  -4.297  -0.920  1.00  0.00
ATOM    157  CB  PRO    11      14.326  -6.068  -1.607  1.00  0.00
ATOM    158  HB1 PRO    11      13.311  -6.399  -1.772  1.00  0.00
ATOM    159  HB2 PRO    11      14.849  -6.791  -0.999  1.00  0.00
ATOM    160  CG  PRO    11      15.036  -5.829  -2.899  1.00  0.00
ATOM    161  HG1 PRO    11      15.582  -6.715  -3.188  1.00  0.00
ATOM    162  HG2 PRO    11      14.324  -5.561  -3.666  1.00  0.00
ATOM    163  CD  PRO    11      15.981  -4.692  -2.646  1.00  0.00
ATOM    164  HD1 PRO    11      16.155  -4.133  -3.552  1.00  0.00
ATOM    165  HD2 PRO    11      16.911  -5.056  -2.237  1.00  0.00
ATOM    166  C   PRO    11      14.732  -4.881   0.572  1.00  0.00
ATOM    167  O   PRO    11      13.991  -5.446   1.375  1.00  0.00
ATOM    168  N   ASP    12      15.926  -4.397   0.912  1.00  0.00
ATOM    169  HN  ASP    12      16.477  -3.954   0.236  1.00  0.00
ATOM    170  CA  ASP    12      16.430  -4.508   2.276  1.00  0.00
ATOM    171  HA  ASP    12      16.402  -5.551   2.554  1.00  0.00
ATOM    172  CB  ASP    12      17.874  -4.008   2.352  1.00  0.00
ATOM    173  HB1 ASP    12      18.146  -3.873   3.389  1.00  0.00
ATOM    174  HB2 ASP    12      17.948  -3.061   1.839  1.00  0.00
ATOM    175  CG  ASP    12      18.856  -4.975   1.721  1.00  0.00
ATOM    176  OD1 ASP    12      18.870  -6.157   2.125  1.00  0.00
ATOM    177  OD2 ASP    12      19.615  -4.549   0.824  1.00  0.00
ATOM    178  C   ASP    12      15.555  -3.719   3.243  1.00  0.00
ATOM    179  O   ASP    12      14.689  -4.282   3.913  1.00  0.00
ATOM    180  N   GLN    13      15.785  -2.412   3.309  1.00  0.00
ATOM    181  HN  GLN    13      16.486  -2.020   2.748  1.00  0.00
ATOM    182  CA  GLN    13      15.012  -1.546   4.191  1.00  0.00
ATOM    183  HA  GLN    13      15.115  -1.923   5.197  1.00  0.00
ATOM    184  CB  GLN    13      15.550  -0.115   4.134  1.00  0.00
ATOM    185  HB1 GLN    13      15.055   0.411   3.331  1.00  0.00
ATOM    186  HB2 GLN    13      16.610  -0.149   3.931  1.00  0.00
ATOM    187  CG  GLN    13      15.336   0.669   5.420  1.00  0.00
ATOM    188  HG1 GLN    13      15.288  -0.025   6.246  1.00  0.00
ATOM    189  HG2 GLN    13      14.403   1.208   5.347  1.00  0.00
ATOM    190  CD  GLN    13      16.450   1.662   5.687  1.00  0.00
ATOM    191  OE1 GLN    13      16.875   2.391   4.790  1.00  0.00
ATOM    192  NE2 GLN    13      16.930   1.695   6.925  1.00  0.00
ATOM    193 HE21 GLN    13      17.651   2.328   7.125  1.00  0.00
ATOM    194 HE22 GLN    13      16.543   1.085   7.587  1.00  0.00
ATOM    195  C   GLN    13      13.538  -1.566   3.807  1.00  0.00
ATOM    196  O   GLN    13      12.658  -1.499   4.666  1.00  0.00
ATOM    197  N   LEU    14      13.278  -1.666   2.509  1.00  0.00
ATOM    198  HN  LEU    14      14.025  -1.723   1.877  1.00  0.00
ATOM    199  CA  LEU    14      11.914  -1.713   1.999  1.00  0.00
ATOM    200  HA  LEU    14      11.445  -0.764   2.212  1.00  0.00
ATOM    201  CB  LEU    14      11.939  -1.932   0.481  1.00  0.00
ATOM    202  HB1 LEU    14      12.218  -1.001   0.012  1.00  0.00
ATOM    203  HB2 LEU    14      12.702  -2.664   0.261  1.00  0.00
ATOM    204  CG  LEU    14      10.625  -2.407  -0.145  1.00  0.00
ATOM    205  HG  LEU    14       9.801  -1.900   0.333  1.00  0.00
ATOM    206  CD1 LEU    14      10.592  -2.066  -1.628  1.00  0.00
ATOM    207 HD11 LEU    14      11.506  -2.403  -2.095  1.00  0.00
ATOM    208 HD12 LEU    14      10.499  -0.997  -1.749  1.00  0.00
ATOM    209 HD13 LEU    14       9.749  -2.556  -2.091  1.00  0.00
ATOM    210  CD2 LEU    14      10.444  -3.902   0.064  1.00  0.00
ATOM    211 HD21 LEU    14      11.402  -4.354   0.275  1.00  0.00
ATOM    212 HD22 LEU    14      10.026  -4.344  -0.828  1.00  0.00
ATOM    213 HD23 LEU    14       9.777  -4.071   0.897  1.00  0.00
ATOM    214  C   LEU    14      11.121  -2.822   2.688  1.00  0.00
ATOM    215  O   LEU    14      10.019  -2.595   3.188  1.00  0.00
ATOM    216  N   TYR    15      11.697  -4.018   2.715  1.00  0.00
ATOM    217  HN  TYR    15      12.579  -4.131   2.303  1.00  0.00
ATOM    218  CA  TYR    15      11.061  -5.167   3.350  1.00  0.00
ATOM    219  HA  TYR    15      10.125  -5.357   2.843  1.00  0.00
ATOM    220  CB  TYR    15      11.964  -6.394   3.218  1.00  0.00
ATOM    221  HB1 TYR    15      12.163  -6.569   2.173  1.00  0.00
ATOM    222  HB2 TYR    15      12.896  -6.200   3.728  1.00  0.00
ATOM    223  CG  TYR    15      11.374  -7.659   3.798  1.00  0.00
ATOM    224  CD1 TYR    15      12.076  -8.408   4.734  1.00  0.00
ATOM    225  HD1 TYR    15      13.051  -8.070   5.053  1.00  0.00
ATOM    226  CD2 TYR    15      10.121  -8.111   3.402  1.00  0.00
ATOM    227  HD2 TYR    15       9.564  -7.543   2.671  1.00  0.00
ATOM    228  CE1 TYR    15      11.542  -9.565   5.268  1.00  0.00
ATOM    229  HE1 TYR    15      12.102 -10.132   5.998  1.00  0.00
ATOM    230  CE2 TYR    15       9.582  -9.269   3.929  1.00  0.00
ATOM    231  HE2 TYR    15       8.606  -9.604   3.610  1.00  0.00
ATOM    232  CZ  TYR    15      10.296  -9.993   4.860  1.00  0.00
ATOM    233  OH  TYR    15       9.761 -11.145   5.388  1.00  0.00
ATOM    234  HH  TYR    15      10.392 -11.863   5.295  1.00  0.00
ATOM    235  C   TYR    15      10.776  -4.888   4.821  1.00  0.00
ATOM    236  O   TYR    15       9.750  -5.307   5.356  1.00  0.00
ATOM    237  N   SER    16      11.694  -4.181   5.471  1.00  0.00
ATOM    238  HN  SER    16      12.487  -3.869   4.989  1.00  0.00
ATOM    239  CA  SER    16      11.535  -3.836   6.878  1.00  0.00
ATOM    240  HA  SER    16      11.318  -4.746   7.420  1.00  0.00
ATOM    241  CB  SER    16      12.824  -3.220   7.425  1.00  0.00
ATOM    242  HB1 SER    16      13.672  -3.768   7.042  1.00  0.00
ATOM    243  HB2 SER    16      12.889  -2.189   7.111  1.00  0.00
ATOM    244  OG  SER    16      12.852  -3.268   8.841  1.00  0.00
ATOM    245  HG  SER    16      13.743  -3.471   9.137  1.00  0.00
ATOM    246  C   SER    16      10.373  -2.867   7.061  1.00  0.00
ATOM    247  O   SER    16       9.746  -2.824   8.120  1.00  0.00
ATOM    248  N   THR    17      10.087  -2.096   6.017  1.00  0.00
ATOM    249  HN  THR    17      10.615  -2.189   5.195  1.00  0.00
ATOM    250  CA  THR    17       8.983  -1.146   6.049  1.00  0.00
ATOM    251  HA  THR    17       8.965  -0.685   7.025  1.00  0.00
ATOM    252  CB  THR    17       9.182  -0.061   4.982  1.00  0.00
ATOM    253  HB  THR    17       9.395  -0.537   4.037  1.00  0.00
ATOM    254  OG1 THR    17      10.278   0.771   5.316  1.00  0.00
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ATOM    255  HG1 THR    17      10.098   1.223   6.144  1.00  0.00
ATOM    256  CG2 THR    17       7.971   0.832   4.783  1.00  0.00
ATOM    257 HG21 THR    17       7.078   0.224   4.720  1.00  0.00
ATOM    258 HG22 THR    17       8.088   1.395   3.867  1.00  0.00
ATOM    259 HG23 THR    17       7.883   1.513   5.616  1.00  0.00
ATOM    260  C   THR    17       7.662  -1.866   5.821  1.00  0.00
ATOM    261  O   THR    17       6.756  -1.792   6.646  1.00  0.00
ATOM    262  N   LEU    18       7.574  -2.569   4.697  1.00  0.00
ATOM    263  HN  LEU    18       8.339  -2.578   4.083  1.00  0.00
ATOM    264  CA  LEU    18       6.369  -3.302   4.330  1.00  0.00
ATOM    265  HA  LEU    18       5.555  -2.597   4.289  1.00  0.00
ATOM    266  CB  LEU    18       6.550  -3.928   2.955  1.00  0.00
ATOM    267  HB1 LEU    18       7.307  -4.694   3.026  1.00  0.00
ATOM    268  HB2 LEU    18       5.619  -4.389   2.661  1.00  0.00
ATOM    269  CG  LEU    18       6.964  -2.940   1.875  1.00  0.00
ATOM    270  HG  LEU    18       7.969  -2.603   2.075  1.00  0.00
ATOM    271  CD1 LEU    18       6.954  -3.607   0.510  1.00  0.00
ATOM    272 HD11 LEU    18       7.945  -3.963   0.274  1.00  0.00
ATOM    273 HD12 LEU    18       6.640  -2.894  -0.236  1.00  0.00
ATOM    274 HD13 LEU    18       6.270  -4.442   0.524  1.00  0.00
ATOM    275  CD2 LEU    18       6.048  -1.722   1.899  1.00  0.00
ATOM    276 HD21 LEU    18       5.138  -1.963   2.430  1.00  0.00
ATOM    277 HD22 LEU    18       5.811  -1.428   0.889  1.00  0.00
ATOM    278 HD23 LEU    18       6.549  -0.908   2.401  1.00  0.00
ATOM    279  C   LEU    18       6.037  -4.376   5.349  1.00  0.00
ATOM    280  O   LEU    18       4.961  -4.372   5.942  1.00  0.00
ATOM    281  N   LYS    19       6.956  -5.310   5.541  1.00  0.00
ATOM    282  HN  LYS    19       7.802  -5.262   5.048  1.00  0.00
ATOM    283  CA  LYS    19       6.753  -6.372   6.514  1.00  0.00
ATOM    284  HA  LYS    19       5.946  -6.995   6.158  1.00  0.00
ATOM    285  CB  LYS    19       8.029  -7.225   6.635  1.00  0.00
ATOM    286  HB1 LYS    19       8.522  -7.243   5.674  1.00  0.00
ATOM    287  HB2 LYS    19       7.748  -8.232   6.897  1.00  0.00
ATOM    288  CG  LYS    19       9.033  -6.730   7.669  1.00  0.00
ATOM    289  HG1 LYS    19       8.693  -7.018   8.653  1.00  0.00
ATOM    290  HG2 LYS    19       9.096  -5.653   7.608  1.00  0.00
ATOM    291  CD  LYS    19      10.412  -7.319   7.429  1.00  0.00
ATOM    292  HD1 LYS    19      10.559  -7.440   6.365  1.00  0.00
ATOM    293  HD2 LYS    19      11.156  -6.643   7.823  1.00  0.00
ATOM    294  CE  LYS    19      10.567  -8.671   8.106  1.00  0.00
ATOM    295  HE1 LYS    19       9.987  -9.401   7.560  1.00  0.00
ATOM    296  HE2 LYS    19      10.193  -8.598   9.117  1.00  0.00
ATOM    297  NZ  LYS    19      11.988  -9.115   8.146  1.00  0.00
ATOM    298  HZ1 LYS    19      12.044 -10.147   8.030  1.00  0.00
ATOM    299  HZ2 LYS    19      12.418  -8.855   9.057  1.00  0.00
ATOM    300  HZ3 LYS    19      12.526  -8.661   7.380  1.00  0.00
ATOM    301  C   LYS    19       6.349  -5.772   7.863  1.00  0.00
ATOM    302  O   LYS    19       5.624  -6.390   8.646  1.00  0.00
ATOM    303  N   SER    20       6.797  -4.542   8.100  1.00  0.00
ATOM    304  HN  SER    20       7.346  -4.092   7.419  1.00  0.00
ATOM    305  CA  SER    20       6.482  -3.841   9.336  1.00  0.00
ATOM    306  HA  SER    20       6.548  -4.551  10.141  1.00  0.00
ATOM    307  CB  SER    20       7.481  -2.708   9.581  1.00  0.00
ATOM    308  HB1 SER    20       7.647  -2.171   8.659  1.00  0.00
ATOM    309  HB2 SER    20       8.416  -3.123   9.929  1.00  0.00
ATOM    310  OG  SER    20       6.996  -1.801  10.556  1.00  0.00
ATOM    311  HG  SER    20       7.552  -1.841  11.337  1.00  0.00
ATOM    312  C   SER    20       5.070  -3.288   9.292  1.00  0.00
ATOM    313  O   SER    20       4.188  -3.752  10.016  1.00  0.00
ATOM    314  N   ILE    21       4.851  -2.311   8.423  1.00  0.00
ATOM    315  HN  ILE    21       5.590  -1.989   7.866  1.00  0.00
ATOM    316  CA  ILE    21       3.531  -1.717   8.268  1.00  0.00
ATOM    317  HA  ILE    21       3.312  -1.154   9.164  1.00  0.00
ATOM    318  CB  ILE    21       3.477  -0.752   7.069  1.00  0.00
ATOM    319  HB  ILE    21       2.442  -0.564   6.839  1.00  0.00
ATOM    320  CG1 ILE    21       4.155  -1.368   5.846  1.00  0.00
ATOM    321 HG11 ILE    21       4.819  -0.640   5.404  1.00  0.00
ATOM    322 HG12 ILE    21       4.723  -2.227   6.152  1.00  0.00
ATOM    323  CG2 ILE    21       4.130   0.573   7.427  1.00  0.00
ATOM    324 HG21 ILE    21       3.498   1.385   7.101  1.00  0.00
ATOM    325 HG22 ILE    21       5.089   0.644   6.935  1.00  0.00
ATOM    326 HG23 ILE    21       4.268   0.630   8.496  1.00  0.00
ATOM    327  CD1 ILE    21       3.185  -1.819   4.782  1.00  0.00
ATOM    328 HD11 ILE    21       2.645  -2.684   5.134  1.00  0.00
ATOM    329 HD12 ILE    21       3.729  -2.074   3.885  1.00  0.00
ATOM    330 HD13 ILE    21       2.489  -1.022   4.568  1.00  0.00
ATOM    331  C   ILE    21       2.472  -2.801   8.095  1.00  0.00
ATOM    332  O   ILE    21       1.487  -2.838   8.823  1.00  0.00
ATOM    333  N   LEU    22       2.710  -3.715   7.164  1.00  0.00
ATOM    334  HN  LEU    22       3.520  -3.646   6.622  1.00  0.00
ATOM    335  CA  LEU    22       1.785  -4.812   6.920  1.00  0.00
ATOM    336  HA  LEU    22       0.864  -4.390   6.544  1.00  0.00
ATOM    337  CB  LEU    22       2.361  -5.772   5.874  1.00  0.00
ATOM    338  HB1 LEU    22       1.785  -6.685   5.900  1.00  0.00
ATOM    339  HB2 LEU    22       3.379  -6.000   6.147  1.00  0.00
ATOM    340  CG  LEU    22       2.360  -5.245   4.439  1.00  0.00
ATOM    341  HG  LEU    22       3.054  -4.421   4.365  1.00  0.00
ATOM    342  CD1 LEU    22       2.815  -6.329   3.474  1.00  0.00
ATOM    343 HD11 LEU    22       2.102  -6.416   2.668  1.00  0.00
ATOM    344 HD12 LEU    22       2.885  -7.271   3.997  1.00  0.00
ATOM    345 HD13 LEU    22       3.783  -6.069   3.071  1.00  0.00
ATOM    346  CD2 LEU    22       0.980  -4.733   4.057  1.00  0.00
ATOM    347 HD21 LEU    22       0.926  -3.671   4.243  1.00  0.00
ATOM    348 HD22 LEU    22       0.234  -5.242   4.647  1.00  0.00
ATOM    349 HD23 LEU    22       0.803  -4.924   3.008  1.00  0.00
ATOM    350  C   LEU    22       1.493  -5.568   8.214  1.00  0.00
ATOM    351  O   LEU    22       0.340  -5.862   8.525  1.00  0.00
ATOM    352  N   GLN    23       2.546  -5.868   8.971  1.00  0.00
ATOM    353  HN  GLN    23       3.447  -5.617   8.666  1.00  0.00
ATOM    354  CA  GLN    23       2.402  -6.598  10.226  1.00  0.00
ATOM    355  HA  GLN    23       2.066  -7.596   9.989  1.00  0.00
ATOM    356  CB  GLN    23       3.754  -6.684  10.940  1.00  0.00
ATOM    357  HB1 GLN    23       3.588  -6.635  12.006  1.00  0.00
ATOM    358  HB2 GLN    23       4.360  -5.842  10.640  1.00  0.00
ATOM    359  CG  GLN    23       4.528  -7.958  10.637  1.00  0.00
ATOM    360  HG1 GLN    23       4.592  -8.082   9.566  1.00  0.00
ATOM    361  HG2 GLN    23       5.523  -7.865  11.048  1.00  0.00
ATOM    362  CD  GLN    23       3.875  -9.191  11.231  1.00  0.00
ATOM    363  OE1 GLN    23       3.304  -9.141  12.320  1.00  0.00
ATOM    364  NE2 GLN    23       3.958 -10.308  10.517  1.00  0.00
ATOM    365 HE21 GLN    23       3.545 -11.120  10.879  1.00  0.00
ATOM    366 HE22 GLN    23       4.429 -10.275   9.658  1.00  0.00
ATOM    367  C   GLN    23       1.374  -5.941  11.151  1.00  0.00
ATOM    368  O   GLN    23       0.462  -6.604  11.646  1.00  0.00
ATOM    369  N   GLN    24       1.542  -4.645  11.404  1.00  0.00
ATOM    370  HN  GLN    24       2.303  -4.175  11.002  1.00  0.00
ATOM    371  CA  GLN    24       0.659  -3.920  12.317  1.00  0.00
ATOM    372  HA  GLN    24       0.434  -4.580  13.142  1.00  0.00
ATOM    373  CB  GLN    24       1.369  -2.679  12.863  1.00  0.00
ATOM    374  HB1 GLN    24       2.330  -2.973  13.260  1.00  0.00
ATOM    375  HB2 GLN    24       0.774  -2.258  13.659  1.00  0.00
ATOM    376  CG  GLN    24       1.596  -1.602  11.817  1.00  0.00
ATOM    377  HG1 GLN    24       0.680  -1.044  11.689  1.00  0.00
ATOM    378  HG2 GLN    24       1.860  -2.077  10.885  1.00  0.00
ATOM    379  CD  GLN    24       2.702  -0.638  12.200  1.00  0.00
ATOM    380  OE1 GLN    24       3.210  -0.671  13.320  1.00  0.00
ATOM    381  NE2 GLN    24       3.082   0.227  11.266  1.00  0.00
ATOM    382 HE21 GLN    24       2.633   0.195  10.395  1.00  0.00
ATOM    383 HE22 GLN    24       3.795   0.862  11.486  1.00  0.00
ATOM    384  C   GLN    24      -0.658  -3.511  11.654  1.00  0.00
ATOM    385  O   GLN    24      -1.727  -3.682  12.237  1.00  0.00
ATOM    386  N   VAL    25      -0.577  -2.936  10.456  1.00  0.00
ATOM    387  HN  VAL    25       0.298  -2.811  10.047  1.00  0.00
ATOM    388  CA  VAL    25      -1.769  -2.477   9.743  1.00  0.00
ATOM    389  HA  VAL    25      -2.139  -1.597  10.251  1.00  0.00
ATOM    390  CB  VAL    25      -1.454  -2.085   8.285  1.00  0.00
ATOM    391  HB  VAL    25      -2.344  -1.670   7.845  1.00  0.00
ATOM    392  CG1 VAL    25      -0.364  -1.025   8.239  1.00  0.00
ATOM    393 HG11 VAL    25      -0.774  -0.102   7.858  1.00  0.00
ATOM    394 HG12 VAL    25       0.434  -1.358   7.591  1.00  0.00
ATOM    395 HG13 VAL    25       0.024  -0.863   9.234  1.00  0.00
ATOM    396  CG2 VAL    25      -1.061  -3.301   7.473  1.00  0.00
ATOM    397 HG21 VAL    25      -1.924  -3.934   7.330  1.00  0.00
ATOM    398 HG22 VAL    25      -0.295  -3.848   7.997  1.00  0.00
ATOM    399 HG23 VAL    25      -0.684  -2.982   6.511  1.00  0.00
ATOM    400  C   VAL    25      -2.865  -3.536   9.760  1.00  0.00
ATOM    401  O   VAL    25      -4.042  -3.213   9.907  1.00  0.00
ATOM    402  N   LYS    26      -2.478  -4.805   9.670  1.00  0.00
ATOM    403  HN  LYS    26      -1.525  -5.013   9.579  1.00  0.00
ATOM    404  CA  LYS    26      -3.448  -5.893   9.728  1.00  0.00
ATOM    405  HA  LYS    26      -4.076  -5.827   8.852  1.00  0.00
ATOM    406  CB  LYS    26      -2.739  -7.248   9.740  1.00  0.00
ATOM    407  HB1 LYS    26      -2.064  -7.280  10.582  1.00  0.00
ATOM    408  HB2 LYS    26      -3.479  -8.026   9.853  1.00  0.00
ATOM    409  CG  LYS    26      -1.940  -7.530   8.479  1.00  0.00
ATOM    410  HG1 LYS    26      -2.552  -8.102   7.797  1.00  0.00
ATOM    411  HG2 LYS    26      -1.665  -6.591   8.020  1.00  0.00
ATOM    412  CD  LYS    26      -0.679  -8.317   8.790  1.00  0.00
ATOM    413  HD1 LYS    26      -0.295  -7.995   9.747  1.00  0.00
ATOM    414  HD2 LYS    26       0.054  -8.123   8.020  1.00  0.00
ATOM    415  CE  LYS    26      -0.955  -9.811   8.844  1.00  0.00
ATOM    416  HE1 LYS    26      -0.358 -10.245   9.632  1.00  0.00
ATOM    417  HE2 LYS    26      -2.002  -9.962   9.062  1.00  0.00
ATOM    418  NZ  LYS    26      -0.625 -10.486   7.558  1.00  0.00
ATOM    419  HZ1 LYS    26       0.302 -10.951   7.627  1.00  0.00
ATOM    420  HZ2 LYS    26      -0.595  -9.790   6.787  1.00  0.00
ATOM    421  HZ3 LYS    26      -1.345 -11.203   7.336  1.00  0.00
ATOM    422  C   LYS    26      -4.318  -5.750  10.973  1.00  0.00
ATOM    423  O   LYS    26      -5.496  -6.105  10.969  1.00  0.00
ATOM    424  N   SER    27      -3.724  -5.203  12.029  1.00  0.00
ATOM    425  HN  SER    27      -2.783  -4.928  11.957  1.00  0.00
ATOM    426  CA  SER    27      -4.437  -4.970  13.281  1.00  0.00
ATOM    427  HA  SER    27      -5.407  -5.436  13.209  1.00  0.00
ATOM    428  CB  SER    27      -3.669  -5.585  14.452  1.00  0.00
ATOM    429  HB1 SER    27      -2.861  -4.927  14.735  1.00  0.00
ATOM    430  HB2 SER    27      -3.267  -6.542  14.152  1.00  0.00
ATOM    431  OG  SER    27      -4.514  -5.777  15.573  1.00  0.00
ATOM    432  HG  SER    27      -5.402  -5.986  15.273  1.00  0.00
ATOM    433  C   SER    27      -4.643  -3.481  13.519  1.00  0.00
ATOM    434  O   SER    27      -4.887  -3.052  14.646  1.00  0.00
ATOM    435  N   HIS    28      -4.516  -2.692  12.457  1.00  0.00
ATOM    436  HN  HIS    28      -4.367  -3.088  11.578  1.00  0.00
ATOM    437  CA  HIS    28      -4.755  -1.267  12.552  1.00  0.00
ATOM    438  HA  HIS    28      -4.393  -0.936  13.515  1.00  0.00
ATOM    439  CB  HIS    28      -4.006  -0.512  11.456  1.00  0.00
ATOM    440  HB1 HIS    28      -2.948  -0.628  11.622  1.00  0.00
ATOM    441  HB2 HIS    28      -4.266  -0.930  10.496  1.00  0.00
ATOM    442  CG  HIS    28      -4.292   0.956  11.417  1.00  0.00
ATOM    443  ND1 HIS    28      -4.264   1.759  12.538  1.00  0.00
ATOM    444  HD1 HIS    28      -4.083   1.459  13.454  1.00  0.00
ATOM    445  CD2 HIS    28      -4.569   1.777  10.377  1.00  0.00
ATOM    446  HD2 HIS    28      -4.665   1.487   9.340  1.00  0.00
ATOM    447  CE1 HIS    28      -4.533   3.006  12.191  1.00  0.00
ATOM    448  HE1 HIS    28      -4.587   3.852  12.859  1.00  0.00
ATOM    449  NE2 HIS    28      -4.719   3.042  10.886  1.00  0.00
ATOM    450  HE2 HIS    28      -4.935   3.844  10.367  1.00  0.00
ATOM    451  C   HIS    28      -6.246  -1.009  12.480  1.00  0.00
ATOM    452  O   HIS    28      -6.982  -1.724  11.800  1.00  0.00
ATOM    453  N   GLN    29      -6.690  -0.037  13.241  1.00  0.00
ATOM    454  HN  GLN    29      -6.048   0.472  13.779  1.00  0.00
ATOM    455  CA  GLN    29      -8.109   0.272  13.334  1.00  0.00
ATOM    456  HA  GLN    29      -8.640  -0.668  13.358  1.00  0.00
ATOM    457  CB  GLN    29      -8.371   1.007  14.638  1.00  0.00
ATOM    458  HB1 GLN    29      -9.433   1.018  14.832  1.00  0.00
ATOM    459  HB2 GLN    29      -8.012   2.021  14.552  1.00  0.00
ATOM    460  CG  GLN    29      -7.670   0.341  15.809  1.00  0.00
ATOM    461  HG1 GLN    29      -7.180  -0.560  15.445  1.00  0.00
ATOM    462  HG2 GLN    29      -6.929   1.021  16.203  1.00  0.00
ATOM    463  CD  GLN    29      -8.622  -0.040  16.925  1.00  0.00
ATOM    464  OE1 GLN    29      -8.364   0.234  18.097  1.00  0.00
ATOM    465  NE2 GLN    29      -9.730  -0.676  16.566  1.00  0.00
ATOM    466 HE21 GLN    29      -9.870  -0.861  15.613  1.00  0.00
ATOM    467 HE22 GLN    29     -10.363  -0.935  17.267  1.00  0.00
ATOM    468  C   GLN    29      -8.607   1.069  12.132  1.00  0.00
ATOM    469  O   GLN    29      -9.794   1.378  12.034  1.00  0.00
ATOM    470  N   SER    30      -7.711   1.348  11.191  1.00  0.00
ATOM    471  HN  SER    30      -6.785   1.056  11.306  1.00  0.00
ATOM    472  CA  SER    30      -8.082   2.036   9.965  1.00  0.00
ATOM    473  HA  SER    30      -9.149   2.199   9.989  1.00  0.00
ATOM    474  CB  SER    30      -7.375   3.385   9.874  1.00  0.00
ATOM    475  HB1 SER    30      -6.453   3.269   9.324  1.00  0.00
ATOM    476  HB2 SER    30      -8.013   4.090   9.362  1.00  0.00
ATOM    477  OG  SER    30      -7.079   3.891  11.163  1.00  0.00
ATOM    478  HG  SER    30      -7.871   3.870  11.705  1.00  0.00
ATOM    479  C   SER    30      -7.743   1.184   8.740  1.00  0.00
ATOM    480  O   SER    30      -8.056   1.562   7.611  1.00  0.00
ATOM    481  N   ALA    31      -7.089   0.039   8.962  1.00  0.00
ATOM    482  HN  ALA    31      -6.867  -0.224   9.880  1.00  0.00
ATOM    483  CA  ALA    31      -6.726  -0.855   7.868  1.00  0.00
ATOM    484  HA  ALA    31      -6.413  -0.246   7.034  1.00  0.00
ATOM    485  CB  ALA    31      -5.553  -1.732   8.272  1.00  0.00
ATOM    486  HB1 ALA    31      -5.218  -2.301   7.417  1.00  0.00
ATOM    487  HB2 ALA    31      -5.865  -2.407   9.054  1.00  0.00
ATOM    488  HB3 ALA    31      -4.746  -1.111   8.629  1.00  0.00
ATOM    489  C   ALA    31      -7.906  -1.726   7.433  1.00  0.00
ATOM    490  O   ALA    31      -7.795  -2.496   6.480  1.00  0.00
ATOM    491  N   TRP    32      -9.040  -1.590   8.119  1.00  0.00
ATOM    492  HN  TRP    32      -9.072  -0.974   8.879  1.00  0.00
ATOM    493  CA  TRP    32     -10.222  -2.384   7.799  1.00  0.00
ATOM    494  HA  TRP    32      -9.960  -3.416   7.971  1.00  0.00
ATOM    495  CB  TRP    32     -11.389  -2.030   8.736  1.00  0.00
ATOM    496  HB1 TRP    32     -11.167  -2.390   9.730  1.00  0.00
ATOM    497  HB2 TRP    32     -12.289  -2.507   8.377  1.00  0.00
ATOM    498  CG  TRP    32     -11.644  -0.566   8.823  1.00  0.00
ATOM    499  CD1 TRP    32     -11.330   0.268   9.857  1.00  0.00
ATOM    500  HD1 TRP    32     -10.862  -0.052  10.776  1.00  0.00
ATOM    501  CD2 TRP    32     -12.255   0.241   7.823  1.00  0.00
ATOM    502  NE1 TRP    32     -11.699   1.554   9.549  1.00  0.00
ATOM    503  HE1 TRP    32     -11.582   2.335  10.128  1.00  0.00
ATOM    504  CE2 TRP    32     -12.259   1.564   8.298  1.00  0.00
ATOM    505  CE3 TRP    32     -12.759  -0.025   6.552  1.00  0.00
ATOM    506  HE3 TRP    32     -12.751  -1.026   6.146  1.00  0.00
ATOM    507  CZ2 TRP    32     -12.780   2.612   7.553  1.00  0.00
ATOM    508  HZ2 TRP    32     -12.798   3.627   7.923  1.00  0.00
ATOM    509  CZ3 TRP    32     -13.278   1.012   5.816  1.00  0.00
ATOM    510  HZ3 TRP    32     -13.671   0.827   4.829  1.00  0.00
ATOM    511  CH2 TRP    32     -13.284   2.314   6.317  1.00  0.00
ATOM    512  HH2 TRP    32     -13.669   3.090   5.697  1.00  0.00
ATOM    513  C   TRP    32     -10.647  -2.251   6.323  1.00  0.00
ATOM    514  O   TRP    32     -11.197  -3.202   5.769  1.00  0.00
ATOM    515  N   PRO    33     -10.400  -1.102   5.633  1.00  0.00
ATOM    516  CA  PRO    33     -10.776  -0.964   4.229  1.00  0.00
ATOM    517  HA  PRO    33     -11.746  -1.400   4.038  1.00  0.00
ATOM    518  CB  PRO    33     -10.842   0.550   3.996  1.00  0.00
ATOM    519  HB1 PRO    33     -10.273   0.798   3.113  1.00  0.00
ATOM    520  HB2 PRO    33     -11.870   0.844   3.852  1.00  0.00
ATOM    521  CG  PRO    33     -10.257   1.205   5.213  1.00  0.00
ATOM    522  HG1 PRO    33      -9.438   1.839   4.913  1.00  0.00
ATOM    523  HG2 PRO    33     -11.008   1.791   5.713  1.00  0.00
ATOM    524  CD  PRO    33      -9.749   0.125   6.125  1.00  0.00
ATOM    525  HD1 PRO    33      -8.693   0.063   6.031  1.00  0.00
ATOM    526  HD2 PRO    33     -10.014   0.330   7.146  1.00  0.00
ATOM    527  C   PRO    33      -9.748  -1.604   3.299  1.00  0.00
ATOM    528  O   PRO    33     -10.097  -2.161   2.259  1.00  0.00
ATOM    529  N   PHE    34      -8.481  -1.522   3.688  1.00  0.00
ATOM    530  HN  PHE    34      -8.271  -1.075   4.533  1.00  0.00
ATOM    531  CA  PHE    34      -7.393  -2.109   2.910  1.00  0.00
ATOM    532  HA  PHE    34      -7.546  -1.870   1.872  1.00  0.00
ATOM    533  CB  PHE    34      -6.043  -1.529   3.344  1.00  0.00
ATOM    534  HB1 PHE    34      -5.395  -1.497   2.486  1.00  0.00
ATOM    535  HB2 PHE    34      -5.608  -2.168   4.098  1.00  0.00
ATOM    536  CG  PHE    34      -6.120  -0.134   3.900  1.00  0.00
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ATOM    537  CD1 PHE    34      -6.997   0.794   3.361  1.00  0.00
ATOM    538  HD1 PHE    34      -7.638   0.503   2.542  1.00  0.00
ATOM    539  CD2 PHE    34      -5.300   0.255   4.946  1.00  0.00
ATOM    540  HD2 PHE    34      -4.611  -0.459   5.373  1.00  0.00
ATOM    541  CE1 PHE    34      -7.069   2.077   3.868  1.00  0.00
ATOM    542  HE1 PHE    34      -7.761   2.789   3.443  1.00  0.00
ATOM    543  CE2 PHE    34      -5.368   1.536   5.459  1.00  0.00
ATOM    544  HE2 PHE    34      -4.728   1.824   6.279  1.00  0.00
ATOM    545  CZ  PHE    34      -6.252   2.450   4.917  1.00  0.00
ATOM    546  HZ  PHE    34      -6.304   3.453   5.314  1.00  0.00
ATOM    547  C   PHE    34      -7.400  -3.624   3.053  1.00  0.00
ATOM    548  O   PHE    34      -7.293  -4.349   2.065  1.00  0.00
ATOM    549  N   MET    35      -7.543  -4.100   4.285  1.00  0.00
ATOM    550  HN  MET    35      -7.635  -3.476   5.035  1.00  0.00
ATOM    551  CA  MET    35      -7.587  -5.534   4.541  1.00  0.00
ATOM    552  HA  MET    35      -6.624  -5.948   4.283  1.00  0.00
ATOM    553  CB  MET    35      -7.868  -5.802   6.021  1.00  0.00
ATOM    554  HB1 MET    35      -8.472  -4.998   6.413  1.00  0.00
ATOM    555  HB2 MET    35      -8.415  -6.729   6.110  1.00  0.00
ATOM    556  CG  MET    35      -6.609  -5.910   6.868  1.00  0.00
ATOM    557  HG1 MET    35      -6.714  -5.267   7.730  1.00  0.00
ATOM    558  HG2 MET    35      -5.766  -5.582   6.278  1.00  0.00
ATOM    559  SD  MET    35      -6.296  -7.591   7.437  1.00  0.00
ATOM    560  CE  MET    35      -4.848  -8.011   6.470  1.00  0.00
ATOM    561  HE1 MET    35      -4.248  -8.726   7.013  1.00  0.00
ATOM    562  HE2 MET    35      -4.268  -7.119   6.285  1.00  0.00
ATOM    563  HE3 MET    35      -5.157  -8.441   5.529  1.00  0.00
ATOM    564  C   MET    35      -8.656  -6.194   3.674  1.00  0.00
ATOM    565  O   MET    35      -9.847  -5.924   3.827  1.00  0.00
ATOM    566  N   GLU    36      -8.219  -7.049   2.751  1.00  0.00
ATOM    567  HN  GLU    36      -7.255  -7.208   2.671  1.00  0.00
ATOM    568  CA  GLU    36      -9.128  -7.729   1.829  1.00  0.00
ATOM    569  HA  GLU    36      -8.598  -8.569   1.409  1.00  0.00
ATOM    570  CB  GLU    36     -10.371  -8.248   2.562  1.00  0.00
ATOM    571  HB1 GLU    36     -11.151  -7.504   2.496  1.00  0.00
ATOM    572  HB2 GLU    36     -10.122  -8.406   3.601  1.00  0.00
ATOM    573  CG  GLU    36     -10.907  -9.553   1.996  1.00  0.00
ATOM    574  HG1 GLU    36     -10.073 -10.192   1.748  1.00  0.00
ATOM    575  HG2 GLU    36     -11.473  -9.338   1.102  1.00  0.00
ATOM    576  CD  GLU    36     -11.806 -10.289   2.972  1.00  0.00
ATOM    577  OE1 GLU    36     -11.522 -11.469   3.266  1.00  0.00
ATOM    578  OE2 GLU    36     -12.794  -9.685   3.440  1.00  0.00
ATOM    579  C   GLU    36      -9.543  -6.792   0.696  1.00  0.00
ATOM    580  O   GLU    36     -10.414  -5.939   0.873  1.00  0.00
ATOM    581  N   PRO    37      -8.913  -6.929  -0.486  1.00  0.00
ATOM    582  CA  PRO    37      -9.200  -6.075  -1.644  1.00  0.00
ATOM    583  HA  PRO    37      -9.135  -5.029  -1.386  1.00  0.00
ATOM    584  CB  PRO    37      -8.087  -6.425  -2.646  1.00  0.00
ATOM    585  HB1 PRO    37      -7.650  -5.515  -3.031  1.00  0.00
ATOM    586  HB2 PRO    37      -8.504  -6.999  -3.461  1.00  0.00
ATOM    587  CG  PRO    37      -7.087  -7.224  -1.876  1.00  0.00
ATOM    588  HG1 PRO    37      -6.627  -7.957  -2.522  1.00  0.00
ATOM    589  HG2 PRO    37      -6.338  -6.570  -1.455  1.00  0.00
ATOM    590  CD  PRO    37      -7.857  -7.904  -0.784  1.00  0.00
ATOM    591  HD1 PRO    37      -7.229  -8.071   0.077  1.00  0.00
ATOM    592  HD2 PRO    37      -8.276  -8.834  -1.137  1.00  0.00
ATOM    593  C   PRO    37     -10.569  -6.357  -2.254  1.00  0.00
ATOM    594  O   PRO    37     -11.467  -6.866  -1.584  1.00  0.00
ATOM    595  N   VAL    38     -10.720  -6.015  -3.531  1.00  0.00
ATOM    596  HN  VAL    38      -9.967  -5.610  -4.008  1.00  0.00
ATOM    597  CA  VAL    38     -11.979  -6.221  -4.237  1.00  0.00
ATOM    598  HA  VAL    38     -12.777  -5.845  -3.614  1.00  0.00
ATOM    599  CB  VAL    38     -12.006  -5.450  -5.571  1.00  0.00
ATOM    600  HB  VAL    38     -11.238  -5.856  -6.213  1.00  0.00
ATOM    601  CG1 VAL    38     -11.704  -3.977  -5.342  1.00  0.00
ATOM    602 HG11 VAL    38     -12.002  -3.410  -6.212  1.00  0.00
ATOM    603 HG12 VAL    38     -10.645  -3.848  -5.174  1.00  0.00
ATOM    604 HG13 VAL    38     -12.250  -3.628  -4.479  1.00  0.00
ATOM    605  CG2 VAL    38     -13.347  -5.625  -6.266  1.00  0.00
ATOM    606 HG21 VAL    38     -13.431  -6.636  -6.639  1.00  0.00
ATOM    607 HG22 VAL    38     -13.419  -4.931  -7.090  1.00  0.00
ATOM    608 HG23 VAL    38     -14.145  -5.434  -5.563  1.00  0.00
ATOM    609  C   VAL    38     -12.222  -7.700  -4.513  1.00  0.00
ATOM    610  O   VAL    38     -11.293  -8.508  -4.492  1.00  0.00
ATOM    611  N   LYS    39     -13.477  -8.047  -4.775  1.00  0.00
ATOM    612  HN  LYS    39     -14.173  -7.357  -4.773  1.00  0.00
ATOM    613  CA  LYS    39     -13.850  -9.431  -5.053  1.00  0.00
ATOM    614  HA  LYS    39     -12.960 -10.036  -4.968  1.00  0.00
ATOM    615  CB  LYS    39     -14.898  -9.939  -4.047  1.00  0.00
ATOM    616  HB1 LYS    39     -15.855  -9.996  -4.546  1.00  0.00
ATOM    617  HB2 LYS    39     -14.615 -10.931  -3.727  1.00  0.00
ATOM    618  CG  LYS    39     -15.065  -9.072  -2.804  1.00  0.00
ATOM    619  HG1 LYS    39     -14.989  -8.033  -3.086  1.00  0.00
ATOM    620  HG2 LYS    39     -14.283  -9.315  -2.099  1.00  0.00
ATOM    621  CD  LYS    39     -16.414  -9.301  -2.144  1.00  0.00
ATOM    622  HD1 LYS    39     -17.168  -8.758  -2.693  1.00  0.00
ATOM    623  HD2 LYS    39     -16.640 -10.357  -2.164  1.00  0.00
ATOM    624  CE  LYS    39     -16.415  -8.824  -0.701  1.00  0.00
ATOM    625  HE1 LYS    39     -16.995  -9.516  -0.107  1.00  0.00
ATOM    626  HE2 LYS    39     -15.398  -8.806  -0.340  1.00  0.00
ATOM    627  NZ  LYS    39     -17.002  -7.462  -0.567  1.00  0.00
ATOM    628  HZ1 LYS    39     -17.552  -7.225  -1.417  1.00  0.00
ATOM    629  HZ2 LYS    39     -16.246  -6.758  -0.448  1.00  0.00
ATOM    630  HZ3 LYS    39     -17.630  -7.423   0.261  1.00  0.00
ATOM    631  C   LYS    39     -14.399  -9.563  -6.469  1.00  0.00
ATOM    632  O   LYS    39     -13.886 -10.337  -7.278  1.00  0.00
ATOM    633  N   ARG    40     -15.448  -8.801  -6.759  1.00  0.00
ATOM    634  HN  ARG    40     -15.810  -8.206  -6.070  1.00  0.00
ATOM    635  CA  ARG    40     -16.078  -8.826  -8.074  1.00  0.00
ATOM    636  HA  ARG    40     -15.347  -8.504  -8.800  1.00  0.00
ATOM    637  CB  ARG    40     -16.534 -10.246  -8.417  1.00  0.00
ATOM    638  HB1 ARG    40     -15.676 -10.822  -8.729  1.00  0.00
ATOM    639  HB2 ARG    40     -17.240 -10.197  -9.234  1.00  0.00
ATOM    640  CG  ARG    40     -17.198 -10.968  -7.256  1.00  0.00
ATOM    641  HG1 ARG    40     -18.190 -10.565  -7.115  1.00  0.00
ATOM    642  HG2 ARG    40     -16.612 -10.809  -6.363  1.00  0.00
ATOM    643  CD  ARG    40     -17.305 -12.462  -7.516  1.00  0.00
ATOM    644  HD1 ARG    40     -16.418 -12.788  -8.038  1.00  0.00
ATOM    645  HD2 ARG    40     -18.173 -12.645  -8.133  1.00  0.00
ATOM    646  NE  ARG    40     -17.434 -13.225  -6.277  1.00  0.00
ATOM    647  HE  ARG    40     -17.683 -12.735  -5.466  1.00  0.00
ATOM    648  CZ  ARG    40     -17.235 -14.537  -6.197  1.00  0.00
ATOM    649  NH1 ARG    40     -16.898 -15.225  -7.279  1.00  0.00
ATOM    650 HH11 ARG    40     -16.794 -14.758  -8.157  1.00  0.00
ATOM    651 HH12 ARG    40     -16.748 -16.212  -7.217  1.00  0.00
ATOM    652  NH2 ARG    40     -17.371 -15.160  -5.034  1.00  0.00
ATOM    653 HH21 ARG    40     -17.624 -14.644  -4.216  1.00  0.00
ATOM    654 HH22 ARG    40     -17.220 -16.147  -4.976  1.00  0.00
ATOM    655  C   ARG    40     -17.268  -7.874  -8.116  1.00  0.00
ATOM    656  O   ARG    40     -17.442  -7.122  -9.074  1.00  0.00
ATOM    657  N   THR    41     -18.081  -7.910  -7.065  1.00  0.00
ATOM    658  HN  THR    41     -17.886  -8.530  -6.332  1.00  0.00
ATOM    659  CA  THR    41     -19.252  -7.047  -6.971  1.00  0.00
ATOM    660  HA  THR    41     -19.528  -6.751  -7.973  1.00  0.00
ATOM    661  CB  THR    41     -20.418  -7.806  -6.335  1.00  0.00
ATOM    662  HB  THR    41     -20.623  -8.689  -6.922  1.00  0.00
ATOM    663  OG1 THR    41     -21.586  -7.003  -6.313  1.00  0.00
ATOM    664  HG1 THR    41     -21.499  -6.331  -5.634  1.00  0.00
ATOM    665  CG2 THR    41     -20.139  -8.252  -4.916  1.00  0.00
ATOM    666 HG21 THR    41     -19.793  -7.409  -4.335  1.00  0.00
ATOM    667 HG22 THR    41     -19.381  -9.020  -4.923  1.00  0.00
ATOM    668 HG23 THR    41     -21.045  -8.644  -4.477  1.00  0.00
ATOM    669  C   THR    41     -18.940  -5.797  -6.155  1.00  0.00
ATOM    670  O   THR    41     -19.562  -4.751  -6.338  1.00  0.00
ATOM    671  N   GLU    42     -17.969  -5.915  -5.254  1.00  0.00
ATOM    672  HN  GLU    42     -17.511  -6.776  -5.156  1.00  0.00
ATOM    673  CA  GLU    42     -17.570  -4.797  -4.408  1.00  0.00
ATOM    674  HA  GLU    42     -18.437  -4.480  -3.847  1.00  0.00
ATOM    675  CB  GLU    42     -16.478  -5.238  -3.432  1.00  0.00
ATOM    676  HB1 GLU    42     -15.513  -5.015  -3.864  1.00  0.00
ATOM    677  HB2 GLU    42     -16.556  -6.304  -3.279  1.00  0.00
ATOM    678  CG  GLU    42     -16.561  -4.556  -2.076  1.00  0.00
ATOM    679  HG1 GLU    42     -17.313  -5.054  -1.482  1.00  0.00
ATOM    680  HG2 GLU    42     -16.845  -3.524  -2.224  1.00  0.00
ATOM    681  CD  GLU    42     -15.246  -4.592  -1.323  1.00  0.00
ATOM    682  OE1 GLU    42     -14.293  -3.913  -1.760  1.00  0.00
ATOM    683  OE2 GLU    42     -15.169  -5.300  -0.297  1.00  0.00
ATOM    684  C   GLU    42     -17.072  -3.626  -5.249  1.00  0.00
ATOM    685  O   GLU    42     -17.374  -2.468  -4.959  1.00  0.00
ATOM    686  N   ALA    43     -16.304  -3.935  -6.288  1.00  0.00
ATOM    687  HN  ALA    43     -16.098  -4.877  -6.467  1.00  0.00
ATOM    688  CA  ALA    43     -15.762  -2.908  -7.171  1.00  0.00
ATOM    689  HA  ALA    43     -16.392  -2.035  -7.091  1.00  0.00
ATOM    690  CB  ALA    43     -14.359  -2.518  -6.730  1.00  0.00
ATOM    691  HB1 ALA    43     -14.122  -3.016  -5.801  1.00  0.00
ATOM    692  HB2 ALA    43     -14.310  -1.449  -6.587  1.00  0.00
ATOM    693  HB3 ALA    43     -13.648  -2.813  -7.487  1.00  0.00
ATOM    694  C   ALA    43     -15.753  -3.381  -8.623  1.00  0.00
ATOM    695  O   ALA    43     -14.707  -3.745  -9.159  1.00  0.00
ATOM    696  N   PRO    44     -16.925  -3.378  -9.280  1.00  0.00
ATOM    697  CA  PRO    44     -17.051  -3.815 -10.673  1.00  0.00
ATOM    698  HA  PRO    44     -16.545  -4.754 -10.841  1.00  0.00
ATOM    699  CB  PRO    44     -18.558  -4.006 -10.840  1.00  0.00
ATOM    700  HB1 PRO    44     -18.842  -3.787 -11.859  1.00  0.00
ATOM    701  HB2 PRO    44     -18.824  -5.024 -10.597  1.00  0.00
ATOM    702  CG  PRO    44     -19.165  -3.039  -9.884  1.00  0.00
ATOM    703  HG1 PRO    44     -19.259  -2.070 -10.352  1.00  0.00
ATOM    704  HG2 PRO    44     -20.133  -3.397  -9.564  1.00  0.00
ATOM    705  CD  PRO    44     -18.224  -2.963  -8.711  1.00  0.00
ATOM    706  HD1 PRO    44     -18.173  -1.953  -8.334  1.00  0.00
ATOM    707  HD2 PRO    44     -18.537  -3.642  -7.932  1.00  0.00
ATOM    708  C   PRO    44     -16.532  -2.775 -11.662  1.00  0.00
ATOM    709  O   PRO    44     -16.263  -3.090 -12.821  1.00  0.00
ATOM    710  N   GLY    45     -16.394  -1.536 -11.200  1.00  0.00
ATOM    711  HN  GLY    45     -16.627  -1.340 -10.268  1.00  0.00
ATOM    712  CA  GLY    45     -15.915  -0.473 -12.064  1.00  0.00
ATOM    713  HA1 GLY    45     -15.960  -0.810 -13.089  1.00  0.00
ATOM    714  HA2 GLY    45     -16.560   0.385 -11.950  1.00  0.00
ATOM    715  C   GLY    45     -14.491  -0.059 -11.747  1.00  0.00
ATOM    716  O   GLY    45     -14.134   1.111 -11.883  1.00  0.00
ATOM    717  N   TYR    46     -13.676  -1.020 -11.327  1.00  0.00
ATOM    718  HN  TYR    46     -14.018  -1.934 -11.241  1.00  0.00
ATOM    719  CA  TYR    46     -12.282  -0.748 -10.995  1.00  0.00
ATOM    720  HA  TYR    46     -12.243   0.205 -10.488  1.00  0.00
ATOM    721  CB  TYR    46     -11.739  -1.832 -10.062  1.00  0.00
ATOM    722  HB1 TYR    46     -10.765  -2.142 -10.411  1.00  0.00
ATOM    723  HB2 TYR    46     -12.408  -2.680 -10.078  1.00  0.00
ATOM    724  CG  TYR    46     -11.595  -1.382  -8.625  1.00  0.00
ATOM    725  CD1 TYR    46     -10.623  -1.931  -7.799  1.00  0.00
ATOM    726  HD1 TYR    46      -9.964  -2.690  -8.196  1.00  0.00
ATOM    727  CD2 TYR    46     -12.432  -0.408  -8.095  1.00  0.00
ATOM    728  HD2 TYR    46     -13.194   0.029  -8.724  1.00  0.00
ATOM    729  CE1 TYR    46     -10.487  -1.522  -6.486  1.00  0.00
ATOM    730  HE1 TYR    46      -9.725  -1.960  -5.859  1.00  0.00
ATOM    731  CE2 TYR    46     -12.303   0.007  -6.783  1.00  0.00
ATOM    732  HE2 TYR    46     -12.964   0.766  -6.389  1.00  0.00
ATOM    733  CZ  TYR    46     -11.330  -0.553  -5.983  1.00  0.00
ATOM    734  OH  TYR    46     -11.199  -0.143  -4.676  1.00  0.00
ATOM    735  HH  TYR    46     -10.892  -0.877  -4.139  1.00  0.00
ATOM    736  C   TYR    46     -11.427  -0.671 -12.256  1.00  0.00
ATOM    737  O   TYR    46     -11.940  -0.764 -13.371  1.00  0.00
ATOM    738  N   TYR    47     -10.120  -0.506 -12.072  1.00  0.00
ATOM    739  HN  TYR    47      -9.772  -0.440 -11.159  1.00  0.00
ATOM    740  CA  TYR    47      -9.189  -0.421 -13.195  1.00  0.00
ATOM    741  HA  TYR    47      -8.188  -0.506 -12.800  1.00  0.00
ATOM    742  CB  TYR    47      -9.433  -1.567 -14.181  1.00  0.00
ATOM    743  HB1 TYR    47     -10.224  -1.285 -14.860  1.00  0.00
ATOM    744  HB2 TYR    47      -8.529  -1.748 -14.743  1.00  0.00
ATOM    745  CG  TYR    47      -9.833  -2.862 -13.514  1.00  0.00
ATOM    746  CD1 TYR    47     -10.756  -3.715 -14.105  1.00  0.00
ATOM    747  HD1 TYR    47     -11.188  -3.443 -15.057  1.00  0.00
ATOM    748  CD2 TYR    47      -9.290  -3.229 -12.290  1.00  0.00
ATOM    749  HD2 TYR    47      -8.572  -2.574 -11.818  1.00  0.00
ATOM    750  CE1 TYR    47     -11.124  -4.899 -13.496  1.00  0.00
ATOM    751  HE1 TYR    47     -11.843  -5.550 -13.971  1.00  0.00
ATOM    752  CE2 TYR    47      -9.653  -4.411 -11.674  1.00  0.00
ATOM    753  HE2 TYR    47      -9.219  -4.679 -10.722  1.00  0.00
ATOM    754  CZ  TYR    47     -10.570  -5.242 -12.280  1.00  0.00
ATOM    755  OH  TYR    47     -10.934  -6.421 -11.671  1.00  0.00
ATOM    756  HH  TYR    47     -10.153  -6.958 -11.519  1.00  0.00
ATOM    757  C   TYR    47      -9.318   0.917 -13.916  1.00  0.00
ATOM    758  O   TYR    47      -8.360   1.686 -13.992  1.00  0.00
ATOM    759  N   GLU    48     -10.504   1.184 -14.451  1.00  0.00
ATOM    760  HN  GLU    48     -11.227   0.529 -14.362  1.00  0.00
ATOM    761  CA  GLU    48     -10.754   2.425 -15.175  1.00  0.00
ATOM    762  HA  GLU    48     -10.103   2.441 -16.037  1.00  0.00
ATOM    763  CB  GLU    48     -12.209   2.478 -15.648  1.00  0.00
ATOM    764  HB1 GLU    48     -12.854   2.529 -14.784  1.00  0.00
ATOM    765  HB2 GLU    48     -12.349   3.368 -16.244  1.00  0.00
ATOM    766  CG  GLU    48     -12.621   1.276 -16.482  1.00  0.00
ATOM    767  HG1 GLU    48     -12.135   1.337 -17.444  1.00  0.00
ATOM    768  HG2 GLU    48     -12.304   0.376 -15.976  1.00  0.00
ATOM    769  CD  GLU    48     -14.120   1.204 -16.702  1.00  0.00
ATOM    770  OE1 GLU    48     -14.858   1.919 -15.994  1.00  0.00
ATOM    771  OE2 GLU    48     -14.554   0.433 -17.584  1.00  0.00
ATOM    772  C   GLU    48     -10.445   3.639 -14.306  1.00  0.00
ATOM    773  O   GLU    48     -10.136   4.716 -14.815  1.00  0.00
ATOM    774  N   VAL    49     -10.529   3.459 -12.992  1.00  0.00
ATOM    775  HN  VAL    49     -10.781   2.578 -12.644  1.00  0.00
ATOM    776  CA  VAL    49     -10.261   4.545 -12.055  1.00  0.00
ATOM    777  HA  VAL    49      -9.905   5.392 -12.624  1.00  0.00
ATOM    778  CB  VAL    49     -11.542   4.971 -11.313  1.00  0.00
ATOM    779  HB  VAL    49     -12.308   5.171 -12.047  1.00  0.00
ATOM    780  CG1 VAL    49     -12.033   3.853 -10.407  1.00  0.00
ATOM    781 HG11 VAL    49     -11.630   3.991  -9.414  1.00  0.00
ATOM    782 HG12 VAL    49     -11.705   2.901 -10.799  1.00  0.00
ATOM    783 HG13 VAL    49     -13.112   3.872 -10.364  1.00  0.00
ATOM    784  CG2 VAL    49     -11.301   6.246 -10.518  1.00  0.00
ATOM    785 HG21 VAL    49     -10.706   6.020  -9.646  1.00  0.00
ATOM    786 HG22 VAL    49     -12.249   6.661 -10.209  1.00  0.00
ATOM    787 HG23 VAL    49     -10.779   6.963 -11.135  1.00  0.00
ATOM    788  C   VAL    49      -9.195   4.160 -11.026  1.00  0.00
ATOM    789  O   VAL    49      -8.861   4.956 -10.148  1.00  0.00
ATOM    790  N   ILE    50      -8.665   2.941 -11.130  1.00  0.00
ATOM    791  HN  ILE    50      -8.958   2.347 -11.847  1.00  0.00
ATOM    792  CA  ILE    50      -7.644   2.474 -10.204  1.00  0.00
ATOM    793  HA  ILE    50      -7.342   3.309  -9.589  1.00  0.00
ATOM    794  CB  ILE    50      -8.182   1.365  -9.282  1.00  0.00
ATOM    795  HB  ILE    50      -8.267   0.458  -9.861  1.00  0.00
ATOM    796  CG1 ILE    50      -9.559   1.747  -8.737  1.00  0.00
ATOM    797 HG11 ILE    50     -10.222   1.952  -9.564  1.00  0.00
ATOM    798 HG12 ILE    50      -9.952   0.921  -8.162  1.00  0.00
ATOM    799  CG2 ILE    50      -7.210   1.105  -8.142  1.00  0.00
ATOM    800 HG21 ILE    50      -6.248   1.528  -8.387  1.00  0.00
ATOM    801 HG22 ILE    50      -7.108   0.041  -7.991  1.00  0.00
ATOM    802 HG23 ILE    50      -7.586   1.561  -7.238  1.00  0.00
ATOM    803  CD1 ILE    50      -9.540   2.967  -7.843  1.00  0.00
ATOM    804 HD11 ILE    50      -9.670   3.855  -8.443  1.00  0.00
ATOM    805 HD12 ILE    50      -8.593   3.019  -7.325  1.00  0.00
ATOM    806 HD13 ILE    50     -10.341   2.898  -7.123  1.00  0.00
ATOM    807  C   ILE    50      -6.428   1.945 -10.953  1.00  0.00
ATOM    808  O   ILE    50      -6.557   1.228 -11.945  1.00  0.00
ATOM    809  N   ARG    51      -5.248   2.301 -10.466  1.00  0.00
ATOM    810  HN  ARG    51      -5.216   2.877  -9.676  1.00  0.00
ATOM    811  CA  ARG    51      -4.000   1.873 -11.085  1.00  0.00
ATOM    812  HA  ARG    51      -4.014   2.198 -12.114  1.00  0.00
ATOM    813  CB  ARG    51      -2.811   2.519 -10.373  1.00  0.00
ATOM    814  HB1 ARG    51      -3.181   3.123  -9.557  1.00  0.00
ATOM    815  HB2 ARG    51      -2.177   1.740  -9.975  1.00  0.00
ATOM    816  CG  ARG    51      -1.967   3.403 -11.277  1.00  0.00
ATOM    817  HG1 ARG    51      -2.041   3.037 -12.291  1.00  0.00
ATOM    818  HG2 ARG    51      -0.939   3.358 -10.950  1.00  0.00
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ATOM	819	CD	ARG	51	-2.433	4.849	-11.240	1.00	0.00
ATOM	820	HD1	ARG	51	-2.996	5.010	-10.332	1.00	0.00
ATOM	821	HD2	ARG	51	-1.566	5.493	-11.244	1.00	0.00
ATOM	822	NE	ARG	51	-3.275	5.184	-12.385	1.00	0.00
ATOM	823	HE	ARG	51	-4.217	5.390	-12.212	1.00	0.00
ATOM	824	CZ	ARG	51	-2.832	5.226	-13.638	1.00	0.00
ATOM	825	NH1	ARG	51	-1.562	4.953	-13.904	1.00	0.00
ATOM	826	HH11	ARG	51	-1.231	4.984	-14.846	1.00	0.00
ATOM	827	HH12	ARG	51	-0.936	4.716	-13.161	1.00	0.00
ATOM	828	NH2	ARG	51	-3.659	5.539	-14.626	1.00	0.00
ATOM	829	HH21	ARG	51	-3.323	5.569	-15.568	1.00	0.00
ATOM	830	HH22	ARG	51	-4.617	5.746	-14.430	1.00	0.00
ATOM	831	C	ARG	51	-3.864	0.354	-11.056	1.00	0.00
ATOM	832	O	ARG	51	-4.094	-0.319	-12.061	1.00	0.00
ATOM	833	N	SER	52	-3.479	-0.182	-9.901	1.00	0.00
ATOM	834	HN	SER	52	-3.310	0.403	-9.134	1.00	0.00
ATOM	835	CA	SER	52	-3.307	-1.622	-9.751	1.00	0.00
ATOM	836	HA	SER	52	-3.766	-2.101	-10.603	1.00	0.00
ATOM	837	CB	SER	52	-1.820	-1.980	-9.715	1.00	0.00
ATOM	838	HB1	SER	52	-1.690	-3.005	-10.027	1.00	0.00
ATOM	839	HB2	SER	52	-1.447	-1.860	-8.708	1.00	0.00
ATOM	840	OG	SER	52	-1.072	-1.143	-10.580	1.00	0.00
ATOM	841	HG	SER	52	-0.287	-1.608	-10.877	1.00	0.00
ATOM	842	C	SER	52	-3.993	-2.128	-8.488	1.00	0.00
ATOM	843	O	SER	52	-3.353	-2.308	-7.452	1.00	0.00
ATOM	844	N	PRO	53	-5.310	-2.379	-8.565	1.00	0.00
ATOM	845	CA	PRO	53	-6.087	-2.882	-7.435	1.00	0.00
ATOM	846	HA	PRO	53	-6.390	-2.083	-6.773	1.00	0.00
ATOM	847	CB	PRO	53	-7.313	-3.484	-8.111	1.00	0.00
ATOM	848	HB1	PRO	53	-8.160	-3.415	-7.450	1.00	0.00
ATOM	849	HB2	PRO	53	-7.122	-4.519	-8.355	1.00	0.00
ATOM	850	CG	PRO	53	-7.512	-2.661	-9.337	1.00	0.00
ATOM	851	HG1	PRO	53	-7.963	-3.263	-10.110	1.00	0.00
ATOM	852	HG2	PRO	53	-8.139	-1.812	-9.109	1.00	0.00
ATOM	853	CD	PRO	53	-6.145	-2.197	-9.770	1.00	0.00
ATOM	854	HD1	PRO	53	-5.780	-2.805	-10.584	1.00	0.00
ATOM	855	HD2	PRO	53	-6.176	-1.157	-10.060	1.00	0.00
ATOM	856	C	PRO	53	-5.340	-3.947	-6.639	1.00	0.00
ATOM	857	O	PRO	53	-5.425	-5.137	-6.943	1.00	0.00
ATOM	858	N	MET	54	-4.609	-3.512	-5.619	1.00	0.00
ATOM	859	HN	MET	54	-4.581	-2.552	-5.426	1.00	0.00
ATOM	860	CA	MET	54	-3.850	-4.428	-4.777	1.00	0.00
ATOM	861	HA	MET	54	-4.303	-5.405	-4.859	1.00	0.00
ATOM	862	CB	MET	54	-2.398	-4.508	-5.253	1.00	0.00
ATOM	863	HB1	MET	54	-2.390	-4.624	-6.327	1.00	0.00
ATOM	864	HB2	MET	54	-1.897	-3.587	-4.995	1.00	0.00
ATOM	865	CG	MET	54	-1.615	-5.660	-4.644	1.00	0.00
ATOM	866	HG1	MET	54	-1.472	-5.464	-3.592	1.00	0.00
ATOM	867	HG2	MET	54	-0.653	-5.720	-5.132	1.00	0.00
ATOM	868	SD	MET	54	-2.452	-7.247	-4.826	1.00	0.00
ATOM	869	CE	MET	54	-3.383	-7.311	-3.298	1.00	0.00
ATOM	870	HE1	MET	54	-2.905	-7.997	-2.612	1.00	0.00
ATOM	871	HE2	MET	54	-4.388	-7.650	-3.501	1.00	0.00
ATOM	872	HE3	MET	54	-3.418	-6.327	-2.857	1.00	0.00
ATOM	873	C	MET	54	-3.897	-3.984	-3.320	1.00	0.00
ATOM	874	O	MET	54	-2.937	-3.415	-2.802	1.00	0.00
ATOM	875	N	ASP	55	-5.026	-4.240	-2.667	1.00	0.00
ATOM	876	HN	ASP	55	-5.755	-4.699	-3.134	1.00	0.00
ATOM	877	CA	ASP	55	-5.201	-3.870	-1.269	1.00	0.00
ATOM	878	HA	ASP	55	-4.803	-2.874	-1.139	1.00	0.00
ATOM	879	CB	ASP	55	-6.690	-3.863	-0.906	1.00	0.00
ATOM	880	HB1	ASP	55	-6.811	-3.495	0.102	1.00	0.00
ATOM	881	HB2	ASP	55	-7.075	-4.869	-0.964	1.00	0.00
ATOM	882	CG	ASP	55	-7.506	-2.985	-1.835	1.00	0.00
ATOM	883	OD1	ASP	55	-7.575	-3.302	-3.041	1.00	0.00
ATOM	884	OD2	ASP	55	-8.074	-1.981	-1.357	1.00	0.00
ATOM	885	C	ASP	55	-4.435	-4.826	-0.360	1.00	0.00
ATOM	886	O	ASP	55	-3.578	-5.580	-0.819	1.00	0.00
ATOM	887	N	LEU	56	-4.739	-4.786	0.931	1.00	0.00
ATOM	888	HN	LEU	56	-5.426	-4.163	1.242	1.00	0.00
ATOM	889	CA	LEU	56	-4.069	-5.644	1.898	1.00	0.00
ATOM	890	HA	LEU	56	-3.012	-5.620	1.683	1.00	0.00
ATOM	891	CB	LEU	56	-4.305	-5.115	3.318	1.00	0.00
ATOM	892	HB1	LEU	56	-4.223	-5.939	4.008	1.00	0.00
ATOM	893	HB2	LEU	56	-5.306	-4.729	3.371	1.00	0.00
ATOM	894	CG	LEU	56	-3.343	-4.015	3.770	1.00	0.00
ATOM	895	HG	LEU	56	-3.605	-3.702	4.770	1.00	0.00
ATOM	896	CD1	LEU	56	-3.425	-2.802	2.859	1.00	0.00
ATOM	897	HD11	LEU	56	-3.644	-1.924	3.449	1.00	0.00
ATOM	898	HD12	LEU	56	-4.204	-2.950	2.132	1.00	0.00
ATOM	899	HD13	LEU	56	-2.481	-2.668	2.352	1.00	0.00
ATOM	900	CD2	LEU	56	-1.929	-4.544	3.801	1.00	0.00
ATOM	901	HD21	LEU	56	-1.279	-3.850	3.291	1.00	0.00
ATOM	902	HD22	LEU	56	-1.898	-5.500	3.303	1.00	0.00
ATOM	903	HD23	LEU	56	-1.611	-4.656	4.824	1.00	0.00
ATOM	904	C	LEU	56	-4.568	-7.081	1.773	1.00	0.00
ATOM	905	O	LEU	56	-5.294	-7.404	0.835	1.00	0.00
ATOM	906	N	LYS	57	-4.152	-7.939	2.706	1.00	0.00
ATOM	907	HN	LYS	57	-3.564	-7.617	3.417	1.00	0.00
ATOM	908	CA	LYS	57	-4.555	-9.347	2.715	1.00	0.00
ATOM	909	HA	LYS	57	-4.259	-9.758	3.669	1.00	0.00
ATOM	910	CB	LYS	57	-6.075	-9.490	2.576	1.00	0.00
ATOM	911	HB1	LYS	57	-6.549	-9.007	3.418	1.00	0.00
ATOM	912	HB2	LYS	57	-6.396	-9.008	1.668	1.00	0.00
ATOM	913	CG	LYS	57	-6.542	-10.935	2.530	1.00	0.00
ATOM	914	HG1	LYS	57	-6.160	-11.395	1.629	1.00	0.00
ATOM	915	HG2	LYS	57	-7.622	-10.954	2.517	1.00	0.00
ATOM	916	CD	LYS	57	-6.049	-11.720	3.735	1.00	0.00
ATOM	917	HD1	LYS	57	-5.944	-11.047	4.573	1.00	0.00
ATOM	918	HD2	LYS	57	-5.090	-12.157	3.498	1.00	0.00
ATOM	919	CE	LYS	57	-7.017	-12.831	4.112	1.00	0.00
ATOM	920	HE1	LYS	57	-7.967	-12.640	3.635	1.00	0.00
ATOM	921	HE2	LYS	57	-6.621	-13.771	3.759	1.00	0.00
ATOM	922	NZ	LYS	57	-7.223	-12.915	5.585	1.00	0.00
ATOM	923	HZ1	LYS	57	-6.363	-12.609	6.084	1.00	0.00
ATOM	924	HZ2	LYS	57	-7.441	-13.894	5.860	1.00	0.00
ATOM	925	HZ3	LYS	57	-8.013	-12.302	5.871	1.00	0.00
ATOM	926	C	LYS	57	-3.855	-10.144	1.617	1.00	0.00
ATOM	927	O	LYS	57	-3.197	-11.146	1.895	1.00	0.00
ATOM	928	N	THR	58	-4.014	-9.714	0.370	1.00	0.00
ATOM	929	HN	THR	58	-4.551	-8.913	0.201	1.00	0.00
ATOM	930	CA	THR	58	-3.403	-10.411	-0.755	1.00	0.00
ATOM	931	HA	THR	58	-3.409	-11.465	-0.527	1.00	0.00
ATOM	932	CB	THR	58	-4.223	-10.177	-2.031	1.00	0.00
ATOM	933	HB	THR	58	-4.448	-9.126	-2.112	1.00	0.00
ATOM	934	OG1	THR	58	-5.448	-10.887	-1.970	1.00	0.00
ATOM	935	HG1	THR	58	-5.974	-10.557	-1.238	1.00	0.00
ATOM	936	CG2	THR	58	-3.515	-10.598	-3.304	1.00	0.00
ATOM	937	HG21	THR	58	-4.236	-11.003	-3.999	1.00	0.00
ATOM	938	HG22	THR	58	-2.775	-11.349	-3.073	1.00	0.00
ATOM	939	HG23	THR	58	-3.031	-9.740	-3.747	1.00	0.00
ATOM	940	C	THR	58	-1.956	-9.961	-0.952	1.00	0.00
ATOM	941	O	THR	58	-1.093	-10.759	-1.318	1.00	0.00
ATOM	942	N	MET	59	-1.697	-8.682	-0.701	1.00	0.00
ATOM	943	HN	MET	59	-2.426	-8.092	-0.413	1.00	0.00
ATOM	944	CA	MET	59	-0.355	-8.132	-0.851	1.00	0.00
ATOM	945	HA	MET	59	0.020	-8.431	-1.819	1.00	0.00
ATOM	946	CB	MET	59	-0.404	-6.605	-0.783	1.00	0.00
ATOM	947	HB1	MET	59	0.536	-6.209	-1.138	1.00	0.00
ATOM	948	HB2	MET	59	-1.200	-6.252	-1.423	1.00	0.00
ATOM	949	CG	MET	59	-0.650	-6.072	0.617	1.00	0.00
ATOM	950	HG1	MET	59	-1.503	-6.585	1.032	1.00	0.00
ATOM	951	HG2	MET	59	0.218	-6.279	1.223	1.00	0.00
ATOM	952	SD	MET	59	-0.969	-4.297	0.643	1.00	0.00
ATOM	953	CE	MET	59	0.230	-3.715	-0.554	1.00	0.00
ATOM	954	HE1	MET	59	0.178	-4.324	-1.443	1.00	0.00
ATOM	955	HE2	MET	59	1.221	-3.779	-0.131	1.00	0.00
ATOM	956	HE3	MET	59	0.016	-2.688	-0.808	1.00	0.00
ATOM	957	C	MET	59	0.582	-8.669	0.228	1.00	0.00
ATOM	958	O	MET	59	1.701	-9.092	-0.061	1.00	0.00
ATOM	959	N	SER	60	0.126	-8.621	1.476	1.00	0.00
ATOM	960	HN	SER	60	-0.772	-8.270	1.644	1.00	0.00
ATOM	961	CA	SER	60	0.925	-9.088	2.601	1.00	0.00
ATOM	962	HA	SER	60	1.789	-8.445	2.682	1.00	0.00
ATOM	963	CB	SER	60	0.117	-9.004	3.898	1.00	0.00
ATOM	964	HB1	SER	60	0.214	-8.013	4.315	1.00	0.00
ATOM	965	HB2	SER	60	-0.922	-9.205	3.686	1.00	0.00
ATOM	966	OG	SER	60	0.579	-9.946	4.852	1.00	0.00
ATOM	967	HG	SER	60	1.273	-9.548	5.383	1.00	0.00
ATOM	968	C	SER	60	1.401	-10.517	2.372	1.00	0.00
ATOM	969	O	SER	60	2.417	-10.939	2.923	1.00	0.00
ATOM	970	N	GLU	61	0.665	-11.258	1.551	1.00	0.00
ATOM	971	HN	GLU	61	-0.134	-10.867	1.137	1.00	0.00
ATOM	972	CA	GLU	61	1.022	-12.636	1.249	1.00	0.00
ATOM	973	HA	GLU	61	1.138	-13.156	2.186	1.00	0.00
ATOM	974	CB	GLU	61	-0.084	-13.309	0.435	1.00	0.00
ATOM	975	HB1	GLU	61	0.025	-14.380	0.516	1.00	0.00
ATOM	976	HB2	GLU	61	0.021	-13.022	-0.601	1.00	0.00
ATOM	977	CG	GLU	61	-1.484	-12.937	0.891	1.00	0.00
ATOM	978	HG1	GLU	61	-1.460	-12.730	1.951	1.00	0.00
ATOM	979	HG2	GLU	61	-1.797	-12.051	0.360	1.00	0.00
ATOM	980	CD	GLU	61	-2.493	-14.039	0.636	1.00	0.00
ATOM	981	OE1	GLU	61	-2.755	-14.830	1.567	1.00	0.00
ATOM	982	OE2	GLU	61	-3.020	-14.112	-0.494	1.00	0.00
ATOM	983	C	GLU	61	2.338	-12.695	0.485	1.00	0.00
ATOM	984	O	GLU	61	3.295	-13.334	0.922	1.00	0.00
ATOM	985	N	ARG	62	2.382	-12.013	-0.654	1.00	0.00
ATOM	986	HN	ARG	62	1.588	-11.524	-0.949	1.00	0.00
ATOM	987	CA	ARG	62	3.578	-11.980	-1.479	1.00	0.00
ATOM	988	HA	ARG	62	3.752	-12.979	-1.846	1.00	0.00
ATOM	989	CB	ARG	62	3.368	-11.045	-2.672	1.00	0.00
ATOM	990	HB1	ARG	62	4.330	-10.804	-3.101	1.00	0.00
ATOM	991	HB2	ARG	62	2.898	-10.136	-2.326	1.00	0.00
ATOM	992	CG	ARG	62	2.496	-11.652	-3.761	1.00	0.00
ATOM	993	HG1	ARG	62	1.895	-12.438	-3.328	1.00	0.00
ATOM	994	HG2	ARG	62	3.131	-12.065	-4.528	1.00	0.00
ATOM	995	CD	ARG	62	1.576	-10.619	-4.389	1.00	0.00
ATOM	996	HD1	ARG	62	2.043	-9.647	-4.320	1.00	0.00
ATOM	997	HD2	ARG	62	0.645	-10.609	-3.845	1.00	0.00
ATOM	998	NE	ARG	62	1.299	-10.916	-5.792	1.00	0.00
ATOM	999	HE	ARG	62	1.697	-10.330	-6.467	1.00	0.00
ATOM	1000	CZ	ARG	62	0.541	-11.931	-6.194	1.00	0.00
ATOM	1001	NH1	ARG	62	0.336	-12.136	-7.488	1.00	0.00
ATOM	1002	HH11	ARG	62	0.753	-11.527	-8.163	1.00	0.00
ATOM	1003	HH12	ARG	62	-0.235	-12.900	-7.789	1.00	0.00
ATOM	1004	NH2	ARG	62	-0.014	-12.742	-5.303	1.00	0.00
ATOM	1005	HH21	ARG	62	0.139	-12.590	-4.326	1.00	0.00
ATOM	1006	HH22	ARG	62	-0.583	-13.505	-5.608	1.00	0.00
ATOM	1007	C	ARG	62	4.790	-11.542	-0.664	1.00	0.00
ATOM	1008	O	ARG	62	5.781	-12.266	-0.576	1.00	0.00
ATOM	1009	N	LEU	63	4.700	-10.366	-0.052	1.00	0.00
ATOM	1010	HN	LEU	63	3.882	-9.835	-0.149	1.00	0.00
ATOM	1011	CA	LEU	63	5.792	-9.853	0.768	1.00	0.00
ATOM	1012	HA	LEU	63	6.634	-9.663	0.117	1.00	0.00
ATOM	1013	CB	LEU	63	5.384	-8.546	1.450	1.00	0.00
ATOM	1014	HB1	LEU	63	5.208	-7.805	0.685	1.00	0.00
ATOM	1015	HB2	LEU	63	4.460	-8.716	1.982	1.00	0.00
ATOM	1016	CG	LEU	63	6.413	-7.984	2.436	1.00	0.00
ATOM	1017	HG	LEU	63	7.141	-8.747	2.663	1.00	0.00
ATOM	1018	CD1	LEU	63	7.148	-6.804	1.825	1.00	0.00
ATOM	1019	HD11	LEU	63	6.457	-5.991	1.672	1.00	0.00
ATOM	1020	HD12	LEU	63	7.575	-7.097	0.877	1.00	0.00
ATOM	1021	HD13	LEU	63	7.937	-6.487	2.492	1.00	0.00
ATOM	1022	CD2	LEU	63	5.741	-7.580	3.738	1.00	0.00
ATOM	1023	HD21	LEU	63	4.709	-7.899	3.726	1.00	0.00
ATOM	1024	HD22	LEU	63	5.785	-6.507	3.848	1.00	0.00
ATOM	1025	HD23	LEU	63	6.252	-8.049	4.565	1.00	0.00
ATOM	1026	C	LEU	63	6.204	-10.880	1.817	1.00	0.00
ATOM	1027	O	LEU	63	7.391	-11.134	2.019	1.00	0.00
ATOM	1028	N	LYS	64	5.212	-11.475	2.475	1.00	0.00
ATOM	1029	HN	LYS	64	4.287	-11.235	2.262	1.00	0.00
ATOM	1030	CA	LYS	64	5.469	-12.487	3.492	1.00	0.00
ATOM	1031	HA	LYS	64	5.942	-12.002	4.333	1.00	0.00
ATOM	1032	CB	LYS	64	4.155	-13.122	3.953	1.00	0.00
ATOM	1033	HB1	LYS	64	3.506	-13.240	3.098	1.00	0.00
ATOM	1034	HB2	LYS	64	4.365	-14.094	4.372	1.00	0.00
ATOM	1035	CG	LYS	64	3.416	-12.301	5.000	1.00	0.00
ATOM	1036	HG1	LYS	64	3.615	-11.254	4.828	1.00	0.00
ATOM	1037	HG2	LYS	64	2.356	-12.488	4.907	1.00	0.00
ATOM	1038	CD	LYS	64	3.859	-12.663	6.408	1.00	0.00
ATOM	1039	HD1	LYS	64	3.007	-13.038	6.957	1.00	0.00
ATOM	1040	HD2	LYS	64	4.618	-13.428	6.351	1.00	0.00
ATOM	1041	CE	LYS	64	4.426	-11.459	7.141	1.00	0.00
ATOM	1042	HE1	LYS	64	4.711	-10.712	6.414	1.00	0.00
ATOM	1043	HE2	LYS	64	3.663	-11.056	7.790	1.00	0.00
ATOM	1044	NZ	LYS	64	5.618	-11.817	7.959	1.00	0.00
ATOM	1045	HZ1	LYS	64	6.086	-12.655	7.560	1.00	0.00
ATOM	1046	HZ2	LYS	64	5.332	-12.025	8.936	1.00	0.00
ATOM	1047	HZ3	LYS	64	6.295	-11.028	7.968	1.00	0.00
ATOM	1048	C	LYS	64	6.407	-13.562	2.953	1.00	0.00
ATOM	1049	O	LYS	64	7.255	-14.082	3.677	1.00	0.00
ATOM	1050	N	ASN	65	6.256	-13.879	1.671	1.00	0.00
ATOM	1051	HN	ASN	65	5.569	-13.420	1.143	1.00	0.00
ATOM	1052	CA	ASN	65	7.103	-14.872	1.023	1.00	0.00
ATOM	1053	HA	ASN	65	7.632	-15.410	1.795	1.00	0.00
ATOM	1054	CB	ASN	65	6.254	-15.855	0.214	1.00	0.00
ATOM	1055	HB1	ASN	65	6.762	-16.082	-0.712	1.00	0.00
ATOM	1056	HB2	ASN	65	5.299	-15.400	-0.006	1.00	0.00
ATOM	1057	CG	ASN	65	6.006	-17.155	0.954	1.00	0.00
ATOM	1058	OD1	ASN	65	6.266	-18.239	0.433	1.00	0.00
ATOM	1059	ND2	ASN	65	5.501	-17.052	2.178	1.00	0.00
ATOM	1060	HD21	ASN	65	5.318	-16.156	2.530	1.00	0.00
ATOM	1061	HD22	ASN	65	5.331	-17.877	2.679	1.00	0.00
ATOM	1062	C	ASN	65	8.122	-14.195	0.119	1.00	0.00
ATOM	1063	O	ASN	65	8.532	-14.749	-0.901	1.00	0.00
ATOM	1064	N	ARG	66	8.535	-12.995	0.510	1.00	0.00
ATOM	1065	HN	ARG	66	8.174	-12.614	1.338	1.00	0.00
ATOM	1066	CA	ARG	66	9.524	-12.235	-0.247	1.00	0.00
ATOM	1067	HA	ARG	66	9.535	-11.232	0.148	1.00	0.00
ATOM	1068	CB	ARG	66	10.919	-12.848	-0.092	1.00	0.00
ATOM	1069	HB1	ARG	66	11.122	-13.471	-0.950	1.00	0.00
ATOM	1070	HB2	ARG	66	11.643	-12.051	-0.063	1.00	0.00
ATOM	1071	CG	ARG	66	11.100	-13.692	1.161	1.00	0.00
ATOM	1072	HG1	ARG	66	11.963	-14.321	1.031	1.00	0.00
ATOM	1073	HG2	ARG	66	10.225	-14.307	1.303	1.00	0.00
ATOM	1074	CD	ARG	66	11.298	-12.825	2.392	1.00	0.00
ATOM	1075	HD1	ARG	66	11.969	-12.017	2.143	1.00	0.00
ATOM	1076	HD2	ARG	66	10.342	-12.420	2.689	1.00	0.00
ATOM	1077	NE	ARG	66	11.860	-13.580	3.509	1.00	0.00
ATOM	1078	HE	ARG	66	12.826	-13.512	3.663	1.00	0.00
ATOM	1079	CZ	ARG	66	11.136	-14.344	4.319	1.00	0.00
ATOM	1080	NH1	ARG	66	11.719	-14.998	5.314	1.00	0.00
ATOM	1081	HH11	ARG	66	12.706	-14.917	5.455	1.00	0.00
ATOM	1082	HH12	ARG	66	11.173	-15.573	5.923	1.00	0.00
ATOM	1083	NH2	ARG	66	9.827	-14.454	4.136	1.00	0.00
ATOM	1084	HH21	ARG	66	9.384	-13.963	3.387	1.00	0.00
ATOM	1085	HH22	ARG	66	9.284	-15.030	4.747	1.00	0.00
ATOM	1086	C	ARG	66	9.153	-12.177	-1.725	1.00	0.00
ATOM	1087	O	ARG	66	10.018	-12.041	-2.590	1.00	0.00
ATOM	1088	N	TYR	67	7.862	-12.285	-2.002	1.00	0.00
ATOM	1089	HN	TYR	67	7.230	-12.408	-1.266	1.00	0.00
ATOM	1090	CA	TYR	67	7.364	-12.275	-3.374	1.00	0.00
ATOM	1091	HA	TYR	67	8.125	-12.708	-4.006	1.00	0.00
ATOM	1092	CB	TYR	67	6.091	-13.117	-3.475	1.00	0.00
ATOM	1093	HB1	TYR	67	6.193	-13.995	-2.856	1.00	0.00
ATOM	1094	HB2	TYR	67	5.259	-12.530	-3.121	1.00	0.00
ATOM	1095	CG	TYR	67	5.767	-13.566	-4.881	1.00	0.00
ATOM	1096	CD1	TYR	67	6.113	-14.835	-5.326	1.00	0.00
ATOM	1097	HD1	TYR	67	6.628	-15.506	-4.654	1.00	0.00
ATOM	1098	CD2	TYR	67	5.107	-12.720	-5.761	1.00	0.00
ATOM	1099	HD2	TYR	67	4.827	-11.731	-5.427	1.00	0.00
ATOM	1100	CE1	TYR	67	5.811	-15.247	-6.611	1.00	0.00

ATOM	1101	HE1	TYR	67	6.089	-16.237	-6.940	1.00	0.00
ATOM	1102	CE2	TYR	67	4.798	-13.123	-7.044	1.00	0.00
ATOM	1103	HE2	TYR	67	4.281	-12.449	-7.711	1.00	0.00
ATOM	1104	CZ	TYR	67	5.153	-14.387	-7.466	1.00	0.00
ATOM	1105	OH	TYR	67	4.850	-14.793	-8.745	1.00	0.00
ATOM	1106	HH	TYR	67	4.026	-15.286	-8.737	1.00	0.00
ATOM	1107	C	TYR	67	7.066	-10.860	-3.859	1.00	0.00
ATOM	1108	O	TYR	67	6.990	-10.616	-5.063	1.00	0.00
ATOM	1109	N	TYR	68	6.859	-9.937	-2.925	1.00	0.00
ATOM	1110	HN	TYR	68	6.909	-10.187	-1.978	1.00	0.00
ATOM	1111	CA	TYR	68	6.515	-8.568	-3.280	1.00	0.00
ATOM	1112	HA	TYR	68	6.570	-8.478	-4.355	1.00	0.00
ATOM	1113	CB	TYR	68	5.089	-8.263	-2.821	1.00	0.00
ATOM	1114	HB1	TYR	68	4.746	-9.065	-2.186	1.00	0.00
ATOM	1115	HB2	TYR	68	5.096	-7.348	-2.256	1.00	0.00
ATOM	1116	CG	TYR	68	4.089	-8.103	-3.946	1.00	0.00
ATOM	1117	CD1	TYR	68	4.278	-8.729	-5.174	1.00	0.00
ATOM	1118	HD1	TYR	68	5.157	-9.336	-5.327	1.00	0.00
ATOM	1119	CD2	TYR	68	2.946	-7.334	-3.772	1.00	0.00
ATOM	1120	HD2	TYR	68	2.783	-6.844	-2.823	1.00	0.00
ATOM	1121	CE1	TYR	68	3.359	-8.582	-6.196	1.00	0.00
ATOM	1122	HE1	TYR	68	3.523	-9.075	-7.143	1.00	0.00
ATOM	1123	CE2	TYR	68	2.022	-7.185	-4.789	1.00	0.00
ATOM	1124	HE2	TYR	68	1.141	-6.581	-4.633	1.00	0.00
ATOM	1125	CZ	TYR	68	2.233	-7.811	-5.998	1.00	0.00
ATOM	1126	OH	TYR	68	1.315	-7.665	-7.012	1.00	0.00
ATOM	1127	HH	TYR	68	0.444	-7.518	-6.637	1.00	0.00
ATOM	1128	C	TYR	68	7.484	-7.570	-2.656	1.00	0.00
ATOM	1129	O	TYR	68	7.096	-6.457	-2.303	1.00	0.00
ATOM	1130	N	VAL	69	8.744	-7.967	-2.529	1.00	0.00
ATOM	1131	HN	VAL	69	9.000	-8.862	-2.835	1.00	0.00
ATOM	1132	CA	VAL	69	9.761	-7.086	-1.962	1.00	0.00
ATOM	1133	HA	VAL	69	9.284	-6.461	-1.221	1.00	0.00
ATOM	1134	CB	VAL	69	10.907	-7.854	-1.276	1.00	0.00
ATOM	1135	HB	VAL	69	11.715	-7.964	-1.984	1.00	0.00
ATOM	1136	CG1	VAL	69	10.465	-9.242	-0.846	1.00	0.00
ATOM	1137	HG11	VAL	69	9.487	-9.183	-0.393	1.00	0.00
ATOM	1138	HG12	VAL	69	11.171	-9.640	-0.133	1.00	0.00
ATOM	1139	HG13	VAL	69	10.423	-9.887	-1.712	1.00	0.00
ATOM	1140	CG2	VAL	69	11.422	-7.059	-0.090	1.00	0.00
ATOM	1141	HG21	VAL	69	12.197	-7.619	0.411	1.00	0.00
ATOM	1142	HG22	VAL	69	10.608	-6.872	0.597	1.00	0.00
ATOM	1143	HG23	VAL	69	11.822	-6.118	-0.438	1.00	0.00
ATOM	1144	C	VAL	69	10.352	-6.199	-3.043	1.00	0.00
ATOM	1145	O	VAL	69	11.543	-6.272	-3.345	1.00	0.00
ATOM	1146	N	SER	70	9.507	-5.372	-3.634	1.00	0.00
ATOM	1147	HN	SER	70	8.566	-5.371	-3.359	1.00	0.00
ATOM	1148	CA	SER	70	9.934	-4.491	-4.703	1.00	0.00
ATOM	1149	HA	SER	70	10.985	-4.285	-4.564	1.00	0.00
ATOM	1150	CB	SER	70	9.734	-5.190	-6.045	1.00	0.00
ATOM	1151	HB1	SER	70	10.626	-5.749	-6.289	1.00	0.00
ATOM	1152	HB2	SER	70	8.898	-5.868	-5.966	1.00	0.00
ATOM	1153	OG	SER	70	9.476	-4.258	-7.081	1.00	0.00
ATOM	1154	HG	SER	70	10.175	-3.600	-7.102	1.00	0.00
ATOM	1155	C	SER	70	9.164	-3.179	-4.657	1.00	0.00
ATOM	1156	O	SER	70	7.969	-3.158	-4.359	1.00	0.00
ATOM	1157	N	LYS	71	9.861	-2.083	-4.924	1.00	0.00
ATOM	1158	HN	LYS	71	10.816	-2.163	-5.131	1.00	0.00
ATOM	1159	CA	LYS	71	9.258	-0.761	-4.863	1.00	0.00
ATOM	1160	HA	LYS	71	8.988	-0.582	-3.832	1.00	0.00
ATOM	1161	CB	LYS	71	10.271	0.305	-5.297	1.00	0.00
ATOM	1162	HB1	LYS	71	11.076	0.332	-4.577	1.00	0.00
ATOM	1163	HB2	LYS	71	10.673	0.029	-6.261	1.00	0.00
ATOM	1164	CG	LYS	71	9.687	1.706	-5.409	1.00	0.00
ATOM	1165	HG1	LYS	71	9.954	2.267	-4.528	1.00	0.00
ATOM	1166	HG2	LYS	71	8.613	1.638	-5.482	1.00	0.00
ATOM	1167	CD	LYS	71	10.218	2.433	-6.634	1.00	0.00
ATOM	1168	HD1	LYS	71	11.033	1.863	-7.054	1.00	0.00
ATOM	1169	HD2	LYS	71	9.424	2.521	-7.360	1.00	0.00
ATOM	1170	CE	LYS	71	10.721	3.824	-6.282	1.00	0.00
ATOM	1171	HE1	LYS	71	11.466	3.737	-5.506	1.00	0.00
ATOM	1172	HE2	LYS	71	9.891	4.412	-5.919	1.00	0.00
ATOM	1173	NZ	LYS	71	11.323	4.511	-7.457	1.00	0.00
ATOM	1174	HZ1	LYS	71	10.580	4.970	-8.023	1.00	0.00
ATOM	1175	HZ2	LYS	71	11.823	3.823	-8.056	1.00	0.00
ATOM	1176	HZ3	LYS	71	12.000	5.234	-7.141	1.00	0.00
ATOM	1177	C	LYS	71	7.984	-0.678	-5.707	1.00	0.00
ATOM	1178	O	LYS	71	6.898	-1.000	-5.224	1.00	0.00
ATOM	1179	N	LYS	72	8.116	-0.244	-6.964	1.00	0.00
ATOM	1180	HN	LYS	72	9.002	0.015	-7.290	1.00	0.00
ATOM	1181	CA	LYS	72	6.963	-0.053	-7.846	1.00	0.00
ATOM	1182	HA	LYS	72	6.511	0.892	-7.580	1.00	0.00
ATOM	1183	CB	LYS	72	7.419	0.008	-9.305	1.00	0.00
ATOM	1184	HB1	LYS	72	8.261	0.680	-9.379	1.00	0.00
ATOM	1185	HB2	LYS	72	7.728	-0.979	-9.615	1.00	0.00
ATOM	1186	CG	LYS	72	6.339	0.491	-10.258	1.00	0.00
ATOM	1187	HG1	LYS	72	6.588	0.174	-11.260	1.00	0.00
ATOM	1188	HG2	LYS	72	5.394	0.057	-9.965	1.00	0.00
ATOM	1189	CD	LYS	72	6.214	2.005	-10.238	1.00	0.00
ATOM	1190	HD1	LYS	72	5.264	2.284	-10.669	1.00	0.00
ATOM	1191	HD2	LYS	72	6.261	2.347	-9.214	1.00	0.00
ATOM	1192	CE	LYS	72	7.329	2.668	-11.031	1.00	0.00
ATOM	1193	HE1	LYS	72	7.643	3.559	-10.508	1.00	0.00
ATOM	1194	HE2	LYS	72	8.160	1.981	-11.102	1.00	0.00
ATOM	1195	NZ	LYS	72	6.889	3.041	-12.403	1.00	0.00
ATOM	1196	HZ1	LYS	72	7.488	3.805	-12.775	1.00	0.00
ATOM	1197	HZ2	LYS	72	5.902	3.366	-12.386	1.00	0.00
ATOM	1198	HZ3	LYS	72	6.961	2.219	-13.037	1.00	0.00
ATOM	1199	C	LYS	72	5.915	-1.152	-7.680	1.00	0.00
ATOM	1200	O	LYS	72	4.723	-0.913	-7.869	1.00	0.00
ATOM	1201	N	LEU	73	6.357	-2.345	-7.305	1.00	0.00
ATOM	1202	HN	LEU	73	7.318	-2.480	-7.168	1.00	0.00
ATOM	1203	CA	LEU	73	5.446	-3.462	-7.101	1.00	0.00
ATOM	1204	HA	LEU	73	4.802	-3.527	-7.966	1.00	0.00
ATOM	1205	CB	LEU	73	6.231	-4.764	-6.964	1.00	0.00
ATOM	1206	HB1	LEU	73	6.470	-4.910	-5.922	1.00	0.00
ATOM	1207	HB2	LEU	73	7.152	-4.656	-7.512	1.00	0.00
ATOM	1208	CG	LEU	73	5.508	-6.014	-7.466	1.00	0.00
ATOM	1209	HG	LEU	73	4.553	-6.094	-6.966	1.00	0.00
ATOM	1210	CD1	LEU	73	6.315	-7.262	-7.145	1.00	0.00
ATOM	1211	HD11	LEU	73	6.321	-7.421	-6.076	1.00	0.00
ATOM	1212	HD12	LEU	73	7.328	-7.136	-7.496	1.00	0.00
ATOM	1213	HD13	LEU	73	5.868	-8.115	-7.633	1.00	0.00
ATOM	1214	CD2	LEU	73	5.247	-5.915	-8.961	1.00	0.00
ATOM	1215	HD21	LEU	73	4.982	-6.889	-9.345	1.00	0.00
ATOM	1216	HD22	LEU	73	6.138	-5.562	-9.459	1.00	0.00
ATOM	1217	HD23	LEU	73	4.437	-5.224	-9.140	1.00	0.00
ATOM	1218	C	LEU	73	4.587	-3.247	-5.861	1.00	0.00
ATOM	1219	O	LEU	73	3.375	-3.053	-5.958	1.00	0.00
ATOM	1220	N	PHE	74	5.218	-3.316	-4.693	1.00	0.00
ATOM	1221	HN	PHE	74	6.184	-3.474	-4.678	1.00	0.00
ATOM	1222	CA	PHE	74	4.513	-3.144	-3.434	1.00	0.00
ATOM	1223	HA	PHE	74	3.549	-3.622	-3.526	1.00	0.00
ATOM	1224	CB	PHE	74	5.290	-3.809	-2.305	1.00	0.00
ATOM	1225	HB1	PHE	74	6.174	-3.224	-2.095	1.00	0.00
ATOM	1226	HB2	PHE	74	5.587	-4.799	-2.614	1.00	0.00
ATOM	1227	CG	PHE	74	4.504	-3.929	-1.033	1.00	0.00
ATOM	1228	CD1	PHE	74	4.062	-5.163	-0.585	1.00	0.00
ATOM	1229	HD1	PHE	74	4.271	-6.043	-1.166	1.00	0.00
ATOM	1230	CD2	PHE	74	4.223	-2.807	-0.277	1.00	0.00
ATOM	1231	HD2	PHE	74	4.578	-1.842	-0.610	1.00	0.00
ATOM	1232	CE1	PHE	74	3.350	-5.272	0.593	1.00	0.00
ATOM	1233	HE1	PHE	74	3.006	-6.238	0.930	1.00	0.00
ATOM	1234	CE2	PHE	74	3.518	-2.911	0.903	1.00	0.00
ATOM	1235	HE2	PHE	74	3.316	-2.029	1.489	1.00	0.00
ATOM	1236	CZ	PHE	74	3.087	-4.144	1.342	1.00	0.00
ATOM	1237	HZ	PHE	74	2.524	-4.223	2.257	1.00	0.00
ATOM	1238	C	PHE	74	4.300	-1.670	-3.113	1.00	0.00
ATOM	1239	O	PHE	74	3.172	-1.236	-2.879	1.00	0.00
ATOM	1240	N	MET	75	5.392	-0.902	-3.095	1.00	0.00
ATOM	1241	HN	MET	75	6.262	-1.309	-3.281	1.00	0.00
ATOM	1242	CA	MET	75	5.324	0.529	-2.788	1.00	0.00
ATOM	1243	HA	MET	75	5.190	0.628	-1.721	1.00	0.00
ATOM	1244	CB	MET	75	6.617	1.240	-3.192	1.00	0.00
ATOM	1245	HB1	MET	75	6.403	2.289	-3.330	1.00	0.00
ATOM	1246	HB2	MET	75	6.964	0.834	-4.124	1.00	0.00
ATOM	1247	CG	MET	75	7.738	1.120	-2.171	1.00	0.00
ATOM	1248	HG1	MET	75	8.668	1.379	-2.652	1.00	0.00
ATOM	1249	HG2	MET	75	7.546	1.818	-1.373	1.00	0.00
ATOM	1250	SD	MET	75	7.907	-0.529	-1.461	1.00	0.00
ATOM	1251	CE	MET	75	7.869	-0.153	0.288	1.00	0.00
ATOM	1252	HE1	MET	75	8.136	-1.036	0.851	1.00	0.00
ATOM	1253	HE2	MET	75	6.875	0.161	0.564	1.00	0.00
ATOM	1254	HE3	MET	75	8.569	0.638	0.506	1.00	0.00
ATOM	1255	C	MET	75	4.136	1.176	-3.488	1.00	0.00
ATOM	1256	O	MET	75	3.495	2.073	-2.942	1.00	0.00
ATOM	1257	N	ALA	76	3.826	0.692	-4.687	1.00	0.00
ATOM	1258	HN	ALA	76	4.346	-0.055	-5.060	1.00	0.00
ATOM	1259	CA	ALA	76	2.659	1.177	-5.404	1.00	0.00
ATOM	1260	HA	ALA	76	2.666	2.259	-5.381	1.00	0.00
ATOM	1261	CB	ALA	76	2.669	0.723	-6.853	1.00	0.00
ATOM	1262	HB1	ALA	76	3.441	1.251	-7.393	1.00	0.00
ATOM	1263	HB2	ALA	76	1.706	0.935	-7.300	1.00	0.00
ATOM	1264	HB3	ALA	76	2.858	-0.338	-6.895	1.00	0.00
ATOM	1265	C	ALA	76	1.409	0.682	-4.714	1.00	0.00
ATOM	1266	O	ALA	76	0.613	1.472	-4.236	1.00	0.00
ATOM	1267	N	ASP	77	1.286	-0.640	-4.600	1.00	0.00
ATOM	1268	HN	ASP	77	1.977	-1.214	-4.989	1.00	0.00
ATOM	1269	CA	ASP	77	0.136	-1.260	-3.941	1.00	0.00
ATOM	1270	HA	ASP	77	-0.692	-1.239	-4.637	1.00	0.00
ATOM	1271	CB	ASP	77	0.454	-2.714	-3.586	1.00	0.00
ATOM	1272	HB1	ASP	77	1.280	-2.736	-2.891	1.00	0.00
ATOM	1273	HB2	ASP	77	-0.413	-3.164	-3.124	1.00	0.00
ATOM	1274	CG	ASP	77	0.831	-3.537	-4.802	1.00	0.00
ATOM	1275	OD1	ASP	77	0.295	-3.261	-5.896	1.00	0.00
ATOM	1276	OD2	ASP	77	1.666	-4.455	-4.661	1.00	0.00
ATOM	1277	C	ASP	77	-0.266	-0.491	-2.685	1.00	0.00
ATOM	1278	O	ASP	77	-1.436	-0.169	-2.498	1.00	0.00
ATOM	1279	N	LEU	78	0.718	-0.155	-1.857	1.00	0.00
ATOM	1280	HN	LEU	78	1.639	-0.417	-2.071	1.00	0.00
ATOM	1281	CA	LEU	78	0.464	0.617	-0.649	1.00	0.00
ATOM	1282	HA	LEU	78	-0.294	0.104	-0.077	1.00	0.00
ATOM	1283	CB	LEU	78	1.744	0.724	0.185	1.00	0.00
ATOM	1284	HB1	LEU	78	1.931	1.768	0.378	1.00	0.00
ATOM	1285	HB2	LEU	78	2.562	0.336	-0.402	1.00	0.00
ATOM	1286	CG	LEU	78	1.726	-0.016	1.529	1.00	0.00
ATOM	1287	HG	LEU	78	2.742	-0.221	1.827	1.00	0.00
ATOM	1288	CD1	LEU	78	0.998	-1.347	1.413	1.00	0.00
ATOM	1289	HD11	LEU	78	-0.066	-1.174	1.360	1.00	0.00
ATOM	1290	HD12	LEU	78	1.222	-1.955	2.277	1.00	0.00
ATOM	1291	HD13	LEU	78	1.327	-1.855	0.521	1.00	0.00
ATOM	1292	CD2	LEU	78	1.094	0.844	2.606	1.00	0.00
ATOM	1293	HD21	LEU	78	1.126	1.880	2.303	1.00	0.00
ATOM	1294	HD22	LEU	78	1.641	0.721	3.529	1.00	0.00
ATOM	1295	HD23	LEU	78	0.068	0.541	2.752	1.00	0.00
ATOM	1296	C	LEU	78	-0.045	2.009	-1.009	1.00	0.00
ATOM	1297	O	LEU	78	-1.164	2.385	-0.657	1.00	0.00
ATOM	1298	N	GLN	79	0.780	2.760	-1.731	1.00	0.00
ATOM	1299	HN	GLN	79	1.649	2.393	-1.995	1.00	0.00
ATOM	1300	CA	GLN	79	0.410	4.097	-2.184	1.00	0.00
ATOM	1301	HA	GLN	79	0.357	4.744	-1.321	1.00	0.00
ATOM	1302	CB	GLN	79	1.478	4.621	-3.154	1.00	0.00
ATOM	1303	HB1	GLN	79	1.727	3.833	-3.850	1.00	0.00
ATOM	1304	HB2	GLN	79	2.362	4.879	-2.591	1.00	0.00
ATOM	1305	CG	GLN	79	1.052	5.840	-3.958	1.00	0.00
ATOM	1306	HG1	GLN	79	0.674	5.507	-4.913	1.00	0.00
ATOM	1307	HG2	GLN	79	0.270	6.356	-3.421	1.00	0.00
ATOM	1308	CD	GLN	79	2.194	6.807	-4.202	1.00	0.00
ATOM	1309	OE1	GLN	79	2.596	7.551	-3.307	1.00	0.00
ATOM	1310	NE2	GLN	79	2.722	6.801	-5.420	1.00	0.00
ATOM	1311	HE21	GLN	79	3.462	7.416	-5.607	1.00	0.00
ATOM	1312	HE22	GLN	79	2.350	6.182	-6.083	1.00	0.00
ATOM	1313	C	GLN	79	-0.953	4.061	-2.870	1.00	0.00
ATOM	1314	O	GLN	79	-1.745	4.997	-2.768	1.00	0.00
ATOM	1315	N	ARG	80	-1.205	2.961	-3.563	1.00	0.00
ATOM	1316	HN	ARG	80	-0.522	2.263	-3.602	1.00	0.00
ATOM	1317	CA	ARG	80	-2.439	2.755	-4.287	1.00	0.00
ATOM	1318	HA	ARG	80	-2.705	3.686	-4.766	1.00	0.00
ATOM	1319	CB	ARG	80	-2.211	1.682	-5.363	1.00	0.00
ATOM	1320	HB1	ARG	80	-1.153	1.505	-5.449	1.00	0.00
ATOM	1321	HB2	ARG	80	-2.686	0.767	-5.059	1.00	0.00
ATOM	1322	CG	ARG	80	-2.725	2.063	-6.740	1.00	0.00
ATOM	1323	HG1	ARG	80	-2.057	2.795	-7.171	1.00	0.00
ATOM	1324	HG2	ARG	80	-2.742	1.180	-7.363	1.00	0.00
ATOM	1325	CD	ARG	80	-4.122	2.649	-6.682	1.00	0.00
ATOM	1326	HD1	ARG	80	-4.422	2.735	-5.653	1.00	0.00
ATOM	1327	HD2	ARG	80	-4.792	1.982	-7.193	1.00	0.00
ATOM	1328	NE	ARG	80	-4.186	3.966	-7.310	1.00	0.00
ATOM	1329	HE	ARG	80	-3.338	4.403	-7.534	1.00	0.00
ATOM	1330	CZ	ARG	80	-5.322	4.595	-7.594	1.00	0.00
ATOM	1331	NH1	ARG	80	-6.486	4.030	-7.305	1.00	0.00
ATOM	1332	HH11	ARG	80	-7.339	4.505	-7.519	1.00	0.00
ATOM	1333	HH12	ARG	80	-6.509	3.129	-6.872	1.00	0.00
ATOM	1334	NH2	ARG	80	-5.294	5.790	-8.168	1.00	0.00
ATOM	1335	HH21	ARG	80	-4.418	6.219	-8.386	1.00	0.00
ATOM	1336	HH22	ARG	80	-6.149	6.263	-8.380	1.00	0.00
ATOM	1337	C	ARG	80	-3.562	2.353	-3.329	1.00	0.00
ATOM	1338	O	ARG	80	-4.715	2.740	-3.513	1.00	0.00
ATOM	1339	N	VAL	81	-3.210	1.620	-2.273	1.00	0.00
ATOM	1340	HN	VAL	81	-2.271	1.367	-2.155	1.00	0.00
ATOM	1341	CA	VAL	81	-4.189	1.231	-1.261	1.00	0.00
ATOM	1342	HA	VAL	81	-4.947	0.630	-1.742	1.00	0.00
ATOM	1343	CB	VAL	81	-3.543	0.387	-0.129	1.00	0.00
ATOM	1344	HB	VAL	81	-2.648	0.893	0.201	1.00	0.00
ATOM	1345	CG1	VAL	81	-3.147	-0.988	-0.645	1.00	0.00
ATOM	1346	HG11	VAL	81	-2.073	-1.089	-0.614	1.00	0.00
ATOM	1347	HG12	VAL	81	-3.491	-1.105	-1.661	1.00	0.00
ATOM	1348	HG13	VAL	81	-3.597	-1.750	-0.023	1.00	0.00
ATOM	1349	CG2	VAL	81	-4.476	0.247	1.070	1.00	0.00
ATOM	1350	HG21	VAL	81	-5.364	-0.291	0.774	1.00	0.00
ATOM	1351	HG22	VAL	81	-4.752	1.228	1.429	1.00	0.00
ATOM	1352	HG23	VAL	81	-3.972	-0.295	1.857	1.00	0.00
ATOM	1353	C	VAL	81	-4.844	2.481	-0.674	1.00	0.00
ATOM	1354	O	VAL	81	-6.050	2.507	-0.427	1.00	0.00
ATOM	1355	N	PHE	82	-4.037	3.515	-0.459	1.00	0.00
ATOM	1356	HN	PHE	82	-3.086	3.434	-0.684	1.00	0.00
ATOM	1357	CA	PHE	82	-4.533	4.774	0.080	1.00	0.00
ATOM	1358	HA	PHE	82	-5.269	4.545	0.837	1.00	0.00
ATOM	1359	CB	PHE	82	-3.390	5.572	0.717	1.00	0.00
ATOM	1360	HB1	PHE	82	-2.807	6.034	-0.065	1.00	0.00
ATOM	1361	HB2	PHE	82	-3.810	6.342	1.348	1.00	0.00
ATOM	1362	CG	PHE	82	-2.455	4.746	1.561	1.00	0.00
ATOM	1363	CD1	PHE	82	-2.850	3.520	2.077	1.00	0.00
ATOM	1364	HD1	PHE	82	-3.841	3.149	1.861	1.00	0.00
ATOM	1365	CD2	PHE	82	-1.180	5.209	1.850	1.00	0.00
ATOM	1366	HD2	PHE	82	-0.862	6.163	1.457	1.00	0.00
ATOM	1367	CE1	PHE	82	-1.988	2.768	2.853	1.00	0.00
ATOM	1368	HE1	PHE	82	-2.307	1.815	3.248	1.00	0.00
ATOM	1369	CE2	PHE	82	-0.316	4.462	2.627	1.00	0.00
ATOM	1370	HE2	PHE	82	0.675	4.834	2.842	1.00	0.00
ATOM	1371	CZ	PHE	82	-0.721	3.242	3.131	1.00	0.00
ATOM	1372	HZ	PHE	82	-0.047	2.659	3.741	1.00	0.00
ATOM	1373	C	PHE	82	-5.194	5.601	-1.016	1.00	0.00
ATOM	1374	O	PHE	82	-6.353	5.997	-0.895	1.00	0.00
ATOM	1375	N	THR	83	-4.450	5.849	-2.089	1.00	0.00
ATOM	1376	HN	THR	83	-3.536	5.499	-2.129	1.00	0.00
ATOM	1377	CA	THR	83	-4.968	6.616	-3.215	1.00	0.00
ATOM	1378	HA	THR	83	-5.151	7.624	-2.875	1.00	0.00
ATOM	1379	CB	THR	83	-3.941	6.649	-4.350	1.00	0.00
ATOM	1380	HB	THR	83	-3.649	5.637	-4.588	1.00	0.00
ATOM	1381	OG1	THR	83	-2.784	7.365	-3.955	1.00	0.00
ATOM	1382	HG1	THR	83	-2.246	6.813	-3.382	1.00	0.00

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ATOM   1383  CG2 THR    83      -4.464   7.286  -5.619  1.00  0.00
ATOM   1384 HG21 THR    83      -3.654   7.404  -6.323  1.00  0.00
ATOM   1385 HG22 THR    83      -4.884   8.255  -5.389  1.00  0.00
ATOM   1386 HG23 THR    83      -5.228   6.656  -6.049  1.00  0.00
ATOM   1387  C   THR    83      -6.278   6.017  -3.711  1.00  0.00
ATOM   1388  O   THR    83      -7.221   6.740  -4.033  1.00  0.00
ATOM   1389  N   ASN    84      -6.333   4.690  -3.756  1.00  0.00
ATOM   1390  HN  ASN    84      -5.550   4.170  -3.476  1.00  0.00
ATOM   1391  CA  ASN    84      -7.533   3.987  -4.190  1.00  0.00
ATOM   1392  HA  ASN    84      -7.822   4.381  -5.153  1.00  0.00
ATOM   1393  CB  ASN    84      -7.250   2.491  -4.321  1.00  0.00
ATOM   1394  HB1 ASN    84      -6.457   2.342  -5.039  1.00  0.00
ATOM   1395  HB2 ASN    84      -6.939   2.107  -3.362  1.00  0.00
ATOM   1396  CG  ASN    84      -8.464   1.707  -4.778  1.00  0.00
ATOM   1397  OD1 ASN    84      -9.459   2.282  -5.218  1.00  0.00
ATOM   1398  ND2 ASN    84      -8.388   0.385  -4.672  1.00  0.00
ATOM   1399 HD21 ASN    84      -7.564  -0.004  -4.312  1.00  0.00
ATOM   1400 HD22 ASN    84      -9.158  -0.147  -4.960  1.00  0.00
ATOM   1401  C   ASN    84      -8.670   4.212  -3.201  1.00  0.00
ATOM   1402  O   ASN    84      -9.656   4.879  -3.514  1.00  0.00
ATOM   1403  N   CYS    85      -8.520   3.657  -2.003  1.00  0.00
ATOM   1404  HN  CYS    85      -7.708   3.142  -1.812  1.00  0.00
ATOM   1405  CA  CYS    85      -9.526   3.808  -0.961  1.00  0.00
ATOM   1406  HA  CYS    85     -10.414   3.280  -1.276  1.00  0.00
ATOM   1407  CB  CYS    85      -9.028   3.205   0.354  1.00  0.00
ATOM   1408  HB1 CYS    85      -9.789   3.329   1.109  1.00  0.00
ATOM   1409  HB2 CYS    85      -8.132   3.724   0.665  1.00  0.00
ATOM  ·1410  SG  CYS    85      -8.635   1.443   0.257  1.00  0.00
ATOM   1411  HG  CYS    85      -9.362   0.955   0.652  1.00  0.00
ATOM   1412  C   CYS    85      -9.873   5.278  -0.759  1.00  0.00
ATOM   1413  O   CYS    85     -10.996   5.613  -0.398  1.00  0.00
ATOM   1414  N   LYS    86      -8.898   6.150  -0.993  1.00  0.00
ATOM   1415  HN  LYS    86      -8.021   5.820  -1.281  1.00  0.00
ATOM   1416  CA  LYS    86      -9.102   7.586  -0.840  1.00  0.00
ATOM   1417  HA  LYS    86      -9.725   7.741   0.029  1.00  0.00
ATOM   1418  CB  LYS    86      -7.758   8.290  -0.623  1.00  0.00
ATOM   1419  HB1 LYS    86      -7.355   7.984   0.330  1.00  0.00
ATOM   1420  HB2 LYS    86      -7.078   7.990  -1.405  1.00  0.00
ATOM   1421  CG  LYS    86      -7.853   9.807  -0.632  1.00  0.00
ATOM   1422  HG1 LYS    86      -8.858  10.091  -0.901  1.00  0.00
ATOM   1423  HG2 LYS    86      -7.625  10.178   0.356  1.00  0.00
ATOM   1424  CD  LYS    86      -6.882  10.424  -1.626  1.00  0.00
ATOM   1425  HD1 LYS    86      -7.437  11.020  -2.334  1.00  0.00
ATOM   1426  HD2 LYS    86      -6.363   9.633  -2.147  1.00  0.00
ATOM   1427  CE  LYS    86      -5.860  11.308  -0.930  1.00  0.00
ATOM   1428  HE1 LYS    86      -5.744  10.970   0.090  1.00  0.00
ATOM   1429  HE2 LYS    86      -4.916  11.221  -1.447  1.00  0.00
ATOM   1430  NZ  LYS    86      -6.276  12.738  -0.922  1.00  0.00
ATOM   1431  HZ1 LYS    86      -6.207  13.125   0.041  1.00  0.00
ATOM   1432  HZ2 LYS    86      -7.260  12.825  -1.249  1.00  0.00
ATOM   1433  HZ3 LYS    86      -5.663  13.292  -1.552  1.00  0.00
ATOM   1434  C   LYS    86      -9.805   8.175  -2.060  1.00  0.00
ATOM   1435  O   LYS    86     -10.579   9.126  -1.943  1.00  0.00
ATOM   1436  N   GLU    87      -9.518   7.615  -3.230  1.00  0.00
ATOM   1437  HN  GLU    87      -8.883   6.869  -3.259  1.00  0.00
ATOM   1438  CA  GLU    87     -10.101   8.103  -4.474  1.00  0.00
ATOM   1439  HA  GLU    87     -10.101   9.183  -4.435  1.00  0.00
ATOM   1440  CB  GLU    87      -9.256   7.649  -5.665  1.00  0.00
ATOM   1441  HB1 GLU    87      -9.884   7.607  -6.542  1.00  0.00
ATOM   1442  HB2 GLU    87      -8.869   6.662  -5.462  1.00  0.00
ATOM   1443  CG  GLU    87      -8.084   8.570  -5.963  1.00  0.00
ATOM   1444  HG1 GLU    87      -7.726   8.989  -5.033  1.00  0.00
ATOM   1445  HG2 GLU    87      -7.296   7.993  -6.424  1.00  0.00
ATOM   1446  CD  GLU    87      -8.460   9.707  -6.893  1.00  0.00
ATOM   1447  OE1 GLU    87      -9.484   9.583  -7.597  1.00  0.00
ATOM   1448  OE2 GLU    87      -7.732  10.721  -6.916  1.00  0.00
ATOM   1449  C   GLU    87     -11.539   7.621  -4.645  1.00  0.00
ATOM   1450  O   GLU    87     -12.422   8.397  -5.010  1.00  0.00
ATOM   1451  N   TYR    88     -11.769   6.338  -4.387  1.00  0.00
ATOM   1452  HN  TYR    88     -11.023   5.763  -4.109  1.00  0.00
ATOM   1453  CA  TYR    88     -13.100   5.757  -4.536  1.00  0.00
ATOM   1454  HA  TYR    88     -13.528   6.144  -5.449  1.00  0.00
ATOM   1455  CB  TYR    88     -13.000   4.234  -4.639  1.00  0.00
ATOM   1456  HB1 TYR    88     -12.032   3.971  -5.040  1.00  0.00
ATOM   1457  HB2 TYR    88     -13.104   3.806  -3.653  1.00  0.00
ATOM   1458  CG  TYR    88     -14.054   3.612  -5.527  1.00  0.00
ATOM   1459  CD1 TYR    88     -15.165   2.982  -4.982  1.00  0.00
ATOM   1460  HD1 TYR    88     -15.273   2.942  -3.908  1.00  0.00
ATOM   1461  CD2 TYR    88     -13.935   3.651  -6.911  1.00  0.00
ATOM   1462  HD2 TYR    88     -13.076   4.136  -7.350  1.00  0.00
ATOM   1463  CE1 TYR    88     -16.130   2.410  -5.790  1.00  0.00
ATOM   1464  HE1 TYR    88     -16.987   1.925  -5.347  1.00  0.00
ATOM   1465  CE2 TYR    88     -14.894   3.081  -7.726  1.00  0.00
ATOM   1466  HE2 TYR    88     -14.785   3.122  -8.800  1.00  0.00
ATOM   1467  CZ  TYR    88     -15.990   2.463  -7.161  1.00  0.00
ATOM   1468  OH  TYR    88     -16.947   1.893  -7.969  1.00  0.00
ATOM   1469  HH  TYR    88     -17.473   2.584  -8.378  1.00  0.00
ATOM   1470  C   TYR    88     -14.010   6.137  -3.368  1.00  0.00
ATOM   1471  O   TYR    88     -14.555   5.265  -2.691  1.00  0.00
ATOM   1472  N   ASN    89     -14.187   7.439  -3.150  1.00  0.00
ATOM   1473  HN  ASN    89     -13.737   8.087  -3.727  1.00  0.00
ATOM   1474  CA  ASN    89     -15.038   7.925  -2.070  1.00  0.00
ATOM   1475  HA  ASN    89     -15.652   7.102  -1.736  1.00  0.00
ATOM   1476  CB  ASN    89     -14.185   8.416  -0.899  1.00  0.00
ATOM   1477  HB1 ASN    89     -14.820   8.581  -0.042  1.00  0.00
ATOM   1478  HB2 ASN    89     -13.706   9.344  -1.173  1.00  0.00
ATOM   1479  CG  ASN    89     -13.113   7.419  -0.517  1.00  0.00
ATOM   1480  OD1 ASN    89     -12.001   7.796  -0.149  1.00  0.00
ATOM   1481  ND2 ASN    89     -13.444   6.136  -0.609  1.00  0.00
ATOM   1482 HD21 ASN    89     -12.769   5.467  -0.377  1.00  0.00
ATOM   1483 HD22 ASN    89     -14.348   5.910  -0.912  1.00  0.00
ATOM   1484  C   ASN    89     -15.944   9.048  -2.552  1.00  0.00
ATOM   1485  O   ASN    89     -15.701  10.222  -2.272  1.00  0.00
ATOM   1486  N   ALA    90     -16.997   8.680  -3.272  1.00  0.00
ATOM   1487  HN  ALA    90     -17.141   7.728  -3.456  1.00  0.00
ATOM   1488  CA  ALA    90     -17.954   9.655  -3.783  1.00  0.00
ATOM   1489  HA  ALA    90     -17.486  10.184  -4.599  1.00  0.00
ATOM   1490  CB  ALA    90     -19.185   8.946  -4.326  1.00  0.00
ATOM   1491  HB1 ALA    90     -19.230   7.944  -3.926  1.00  0.00
ATOM   1492  HB2 ALA    90     -19.128   8.901  -5.404  1.00  0.00
ATOM   1493  HB3 ALA    90     -20.072   9.490  -4.035  1.00  0.00
ATOM   1494  C   ALA    90     -18.356  10.662  -2.705  1.00  0.00
ATOM   1495  O   ALA    90     -18.383  11.868  -2.952  1.00  0.00
ATOM   1496  N   PRO    91     -18.657  10.179  -1.487  1.00  0.00
ATOM   1497  CA  PRO    91     -19.087  11.013  -0.381  1.00  0.00
ATOM   1498  HA  PRO    91     -19.505  11.951  -0.717  1.00  0.00
ATOM   1499  CB  PRO    91     -20.176  10.140   0.237  1.00  0.00
ATOM   1500  HB1 PRO    91     -20.271  10.369   1.289  1.00  0.00
ATOM   1501  HB2 PRO    91     -21.115  10.323  -0.263  1.00  0.00
ATOM   1502  CG  PRO    91     -19.704   8.730   0.022  1.00  0.00
ATOM   1503  HG1 PRO    91     -20.537   8.104  -0.258  1.00  0.00
ATOM   1504  HG2 PRO    91     -19.249   8.358   0.929  1.00  0.00
ATOM   1505  CD  PRO    91     -18.679   8.764  -1.094  1.00  0.00
ATOM   1506  HD1 PRO    91     -17.713   8.452  -0.724  1.00  0.00
ATOM   1507  HD2 PRO    91     -18.988   8.139  -1.919  1.00  0.00
ATOM   1508  C   PRO    91     -17.976  11.268   0.633  1.00  0.00
ATOM   1509  O   PRO    91     -18.242  11.671   1.766  1.00  0.00
ATOM   1510  N   GLU    92     -16.734  11.007   0.234  1.00  0.00
ATOM   1511  HN  GLU    92     -16.582  10.671  -0.674  1.00  0.00
ATOM   1512  CA  GLU    92     -15.596  11.174   1.132  1.00  0.00
ATOM   1513  HA  GLU    92     -14.728  10.745   0.654  1.00  0.00
ATOM   1514  CB  GLU    92     -15.340  12.658   1.408  1.00  0.00
ATOM   1515  HB1 GLU    92     -14.454  12.750   2.020  1.00  0.00
ATOM   1516  HB2 GLU    92     -16.183  13.062   1.949  1.00  0.00
ATOM   1517  CG  GLU    92     -15.139  13.487   0.150  1.00  0.00
ATOM   1518  HG1 GLU    92     -15.062  12.821  -0.696  1.00  0.00
ATOM   1519  HG2 GLU    92     -15.993  14.135   0.021  1.00  0.00
ATOM   1520  CD  GLU    92     -13.888  14.343   0.208  1.00  0.00
ATOM   1521  OE1 GLU    92     -13.118  14.335  -0.775  1.00  0.00
ATOM   1522  OE2 GLU    92     -13.679  15.021   1.236  1.00  0.00
ATOM   1523  C   GLU    92     -15.843  10.432   2.436  1.00  0.00
ATOM   1524  O   GLU    92     -15.529  10.925   3.519  1.00  0.00
ATOM   1525  N   SER    93     -16.427   9.248   2.313  1.00  0.00
ATOM   1526  HN  SER    93     -16.649   8.919   1.417  1.00  0.00
ATOM   1527  CA  SER    93     -16.725   8.412   3.463  1.00  0.00
ATOM   1528  HA  SER    93     -17.495   8.899   4.042  1.00  0.00
ATOM   1529  CB  SER    93     -17.234   7.048   2.986  1.00  0.00
ATOM   1530  HB1 SER    93     -17.222   6.350   3.809  1.00  0.00
ATOM   1531  HB2 SER    93     -18.243   7.152   2.615  1.00  0.00
ATOM   1532  OG  SER    93     -16.418   6.536   1.947  1.00  0.00
ATOM   1533  HG  SER    93     -16.849   6.678   1.101  1.00  0.00
ATOM   1534  C   SER    93     -15.490   8.232   4.335  1.00  0.00
ATOM   1535  O   SER    93     -14.447   8.833   4.082  1.00  0.00
ATOM   1536  N   GLU    94     -15.601   7.370   5.338  1.00  0.00
ATOM   1537  HN  GLU    94     -16.455   6.913   5.485  1.00  0.00
ATOM   1538  CA  GLU    94     -14.485   7.092   6.230  1.00  0.00
ATOM   1539  HA  GLU    94     -14.213   8.017   6.717  1.00  0.00
ATOM   1540  CB  GLU    94     -14.901   6.073   7.292  1.00  0.00
ATOM   1541  HB1 GLU    94     -14.489   5.109   7.031  1.00  0.00
ATOM   1542  HB2 GLU    94     -15.979   6.003   7.305  1.00  0.00
ATOM   1543  CG  GLU    94     -14.430   6.427   8.693  1.00  0.00
ATOM   1544  HG1 GLU    94     -13.574   7.082   8.616  1.00  0.00
ATOM   1545  HG2 GLU    94     -15.229   6.939   9.209  1.00  0.00
ATOM   1546  CD  GLU    94     -14.035   5.207   9.502  1.00  0.00
ATOM   1547  OE1 GLU    94     -13.155   5.336  10.379  1.00  0.00
ATOM   1548  OE2 GLU    94     -14.604   4.123   9.257  1.00  0.00
ATOM   1549  C   GLU    94     -13.274   6.569   5.457  1.00  0.00
ATOM   1550  O   GLU    94     -12.160   6.551   5.979  1.00  0.00
ATOM   1551  N   TYR    95     -13.493   6.137   4.214  1.00  0.00
ATOM   1552  HN  TYR    95     -14.397   6.168   3.841  1.00  0.00
ATOM   1553  CA  TYR    95     -12.412   5.611   3.393  1.00  0.00
ATOM   1554  HA  TYR    95     -11.977   4.775   3.916  1.00  0.00
ATOM   1555  CB  TYR    95     -12.947   5.131   2.045  1.00  0.00
ATOM   1556  HB1 TYR    95     -13.630   5.870   1.653  1.00  0.00
ATOM   1557  HB2 TYR    95     -12.119   5.016   1.365  1.00  0.00
ATOM   1558  CG  TYR    95     -13.678   3.807   2.104  1.00  0.00
ATOM   1559  CD1 TYR    95     -13.724   2.972   0.996  1.00  0.00
ATOM   1560  HD1 TYR    95     -13.227   3.279   0.087  1.00  0.00
ATOM   1561  CD2 TYR    95     -14.325   3.394   3.263  1.00  0.00
ATOM   1562  HD2 TYR    95     -14.303   4.030   4.132  1.00  0.00
ATOM   1563  CE1 TYR    95     -14.390   1.762   1.040  1.00  0.00
ATOM   1564  HE1 TYR    95     -14.413   1.126   0.167  1.00  0.00
ATOM   1565  CE2 TYR    95     -14.994   2.187   3.314  1.00  0.00
ATOM   1566  HE2 TYR    95     -15.487   1.884   4.227  1.00  0.00
ATOM   1567  CZ  TYR    95     -15.023   1.374   2.202  1.00  0.00
ATOM   1568  OH  TYR    95     -15.687   0.170   2.250  1.00  0.00
ATOM   1569  HH  TYR    95     -15.095  -0.534   1.974  1.00  0.00
ATOM   1570  C   TYR    95     -11.338   6.671   3.177  1.00  0.00
ATOM   1571  O   TYR    95     -10.170   6.352   2.951  1.00  0.00
ATOM   1572  N   TYR    96     -11.743   7.934   3.243  1.00  0.00
ATOM   1573  HN  TYR    96     -12.686   8.125   3.432  1.00  0.00
ATOM   1574  CA  TYR    96     -10.816   9.045   3.073  1.00  0.00
ATOM   1575  HA  TYR    96     -10.140   8.795   2.268  1.00  0.00
ATOM   1576  CB  TYR    96     -11.579  10.321   2.712  1.00  0.00
ATOM   1577  HB1 TYR    96     -12.376  10.073   2.027  1.00  0.00
ATOM   1578  HB2 TYR    96     -12.001  10.745   3.611  1.00  0.00
ATOM   1579  CG  TYR    96     -10.717  11.378   2.060  1.00  0.00
ATOM   1580  CD1 TYR    96     -10.257  11.219   0.759  1.00  0.00
ATOM   1581  HD1 TYR    96     -10.524  10.326   0.213  1.00  0.00
ATOM   1582  CD2 TYR    96     -10.364  12.533   2.745  1.00  0.00
ATOM   1583  HD2 TYR    96     -10.714  12.672   3.758  1.00  0.00
ATOM   1584  CE1 TYR    96      -9.471  12.183   0.159  1.00  0.00
ATOM   1585  HE1 TYR    96      -9.120  12.039  -0.852  1.00  0.00
ATOM   1586  CE2 TYR    96      -9.576  13.501   2.152  1.00  0.00
ATOM   1587  HE2 TYR    96      -9.312  14.393   2.701  1.00  0.00
ATOM   1588  CZ  TYR    96      -9.133  13.320   0.859  1.00  0.00
ATOM   1589  OH  TYR    96      -8.347  14.282   0.265  1.00  0.00
ATOM   1590  HH  TYR    96      -8.832  14.690  -0.456  1.00  0.00
ATOM   1591  C   TYR    96     -10.009   9.267   4.346  1.00  0.00
ATOM   1592  O   TYR    96      -8.884   9.764   4.303  1.00  0.00
ATOM   1593  N   LYS    97     -10.593   8.888   5.478  1.00  0.00
ATOM   1594  HN  LYS    97     -11.496   8.503   5.445  1.00  0.00
ATOM   1595  CA  LYS    97      -9.937   9.050   6.771  1.00  0.00
ATOM   1596  HA  LYS    97      -9.515  10.043   6.806  1.00  0.00
ATOM   1597  CB  LYS    97     -10.960   8.901   7.898  1.00  0.00
ATOM   1598  HB1 LYS    97     -11.380   7.906   7.859  1.00  0.00
ATOM   1599  HB2 LYS    97     -10.457   9.033   8.845  1.00  0.00
ATOM   1600  CG  LYS    97     -12.100   9.903   7.820  1.00  0.00
ATOM   1601  HG1 LYS    97     -12.840   9.537   7.124  1.00  0.00
ATOM   1602  HG2 LYS    97     -11.711  10.849   7.473  1.00  0.00
ATOM   1603  CD  LYS    97     -12.756  10.107   9.176  1.00  0.00
ATOM   1604  HD1 LYS    97     -13.665  10.674   9.042  1.00  0.00
ATOM   1605  HD2 LYS    97     -12.990   9.142   9.601  1.00  0.00
ATOM   1606  CE  LYS    97     -11.842  10.857  10.131  1.00  0.00
ATOM   1607  HE1 LYS    97     -10.927  11.105   9.614  1.00  0.00
ATOM   1608  HE2 LYS    97     -11.618  10.218  10.972  1.00  0.00
ATOM   1609  NZ  LYS    97     -12.471  12.111  10.629  1.00  0.00
ATOM   1610  HZ1 LYS    97     -11.831  12.917  10.476  1.00  0.00
ATOM   1611  HZ2 LYS    97     -12.672  12.031  11.646  1.00  0.00
ATOM   1612  HZ3 LYS    97     -13.362  12.289  10.123  1.00  0.00
ATOM   1613  C   LYS    97      -8.816   8.031   6.955  1.00  0.00
ATOM   1614  O   LYS    97      -7.664   8.395   7.189  1.00  0.00
ATOM   1615  N   CYS    98      -9.167   6.753   6.861  1.00  0.00
ATOM   1616  HN  CYS    98     -10.105   6.529   6.684  1.00  0.00
ATOM   1617  CA  CYS    98      -8.203   5.671   7.039  1.00  0.00
ATOM   1618  HA  CYS    98      -7.970   5.609   8.092  1.00  0.00
ATOM   1619  CB  CYS    98      -8.816   4.348   6.588  1.00  0.00
ATOM   1620  HB1 CYS    98      -8.039   3.600   6.531  1.00  0.00
ATOM   1621  HB2 CYS    98      -9.554   4.040   7.311  1.00  0.00
ATOM   1622  SG  CYS    98      -9.627   4.426   4.976  1.00  0.00
ATOM   1623  HG  CYS    98     -10.366   5.034   5.045  1.00  0.00
ATOM   1624  C   CYS    98      -6.914   5.931   6.268  1.00  0.00
ATOM   1625  O   CYS    98      -5.817   5.796   6.814  1.00  0.00
ATOM   1626  N   ALA    99      -7.045   6.278   4.991  1.00  0.00
ATOM   1627  HN  ALA    99      -7.939   6.375   4.607  1.00  0.00
ATOM   1628  CA  ALA    99      -5.885   6.551   4.158  1.00  0.00
ATOM   1629  HA  ALA    99      -5.339   5.629   4.029  1.00  0.00
ATOM   1630  CB  ALA    99      -6.319   7.042   2.785  1.00  0.00
ATOM   1631  HB1 ALA    99      -6.855   6.255   2.275  1.00  0.00
ATOM   1632  HB2 ALA    99      -5.448   7.317   2.209  1.00  0.00
ATOM   1633  HB3 ALA    99      -6.963   7.902   2.897  1.00  0.00
ATOM   1634  C   ALA    99      -4.977   7.570   4.828  1.00  0.00
ATOM   1635  O   ALA    99      -3.764   7.398   4.871  1.00  0.00
ATOM   1636  N   ASN   100      -5.581   8.613   5.379  1.00  0.00
ATOM   1637  HN  ASN   100      -6.555   8.685   5.321  1.00  0.00
ATOM   1638  CA  ASN   100      -4.826   9.660   6.054  1.00  0.00
ATOM   1639  HA  ASN   100      -4.202  10.142   5.316  1.00  0.00
ATOM   1640  CB  ASN   100      -5.778  10.695   6.658  1.00  0.00
ATOM   1641  HB1 ASN   100      -6.720  10.660   6.130  1.00  0.00
ATOM   1642  HB2 ASN   100      -5.943  10.459   7.699  1.00  0.00
ATOM   1643  CG  ASN   100      -5.230  12.106   6.568  1.00  0.00
ATOM   1644  OD1 ASN   100      -5.097  12.798   7.577  1.00  0.00
ATOM   1645  ND2 ASN   100      -4.910  12.541   5.354  1.00  0.00
ATOM   1646 HD21 ASN   100      -4.553  13.449   5.267  1.00  0.00
ATOM   1647 HD22 ASN   100      -5.042  11.934   4.595  1.00  0.00
ATOM   1648  C   ASN   100      -3.935   9.073   7.144  1.00  0.00
ATOM   1649  O   ASN   100      -2.862   9.602   7.434  1.00  0.00
ATOM   1650  N   ILE   101      -4.386   7.975   7.743  1.00  0.00
ATOM   1651  HN  ILE   101      -5.248   7.599   7.467  1.00  0.00
ATOM   1652  CA  ILE   101      -3.630   7.318   8.803  1.00  0.00
ATOM   1653  HA  ILE   101      -3.193   8.088   9.422  1.00  0.00
ATOM   1654  CB  ILE   101      -4.541   6.453   9.691  1.00  0.00
ATOM   1655  HB  ILE   101      -4.890   5.616   9.105  1.00  0.00
ATOM   1656  CG1 ILE   101      -5.743   7.274  10.166  1.00  0.00
ATOM   1657 HG11 ILE   101      -6.325   7.575   9.308  1.00  0.00
ATOM   1658 HG12 ILE   101      -5.387   8.153  10.682  1.00  0.00
ATOM   1659  CG2 ILE   101      -3.761   5.909  10.879  1.00  0.00
ATOM   1660 HG21 ILE   101      -4.431   5.373  11.534  1.00  0.00
ATOM   1661 HG22 ILE   101      -3.308   6.727  11.418  1.00  0.00
ATOM   1662 HG23 ILE   101      -2.990   5.240  10.526  1.00  0.00
ATOM   1663  CD1 ILE   101      -6.658   6.523  11.107  1.00  0.00
ATOM   1664 HD11 ILE   101      -7.168   7.226  11.749  1.00  0.00
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ATOM	1665	HD12	ILE	101	-6.075	5.842	11.709	1.00	0.00
ATOM	1666	HD13	ILE	101	-7.384	5.966	10.534	1.00	0.00
ATOM	1667	C	ILE	101	-2.511	6.457	8.226	1.00	0.00
ATOM	1668	O	ILE	101	-1 335	6 807	8 332	1.00	0.00
ATOM	1669	N	LEU	102	-2 876	5 343	7 590	1 00	0.00
ATOM	1670	HN	LEU	102	-3 829	5.117	7 527	1 00	0 00
ATOM	1671	CA	LEU	102	-1 886	4 457	6 972	1 00	0 00
ATOM	1672	HA	LEU	102	-1 350	3 953	7 763	1.00	0 00
ATOM	1673	CB	LEU	102	-2 569	3 416	6.082	1.00	0 00
ATOM	1674	HB1	LEU	102	-3 630	3 443	6.283	1 00	0.00
ATOM	1675	HB2	LEU	102	-2 408	3 700	5 053	1.00	0 00
ATOM	1676	CG	LEU	102	-2 083	1 971	6 260	1 00	0.00
ATOM	1677	HG	LEU	102	-2 423	1 382	5.420	1 00	0 00
ATOM	1678	CD1	LEU	102	-2 676	1 364	7.523	1 00	0 00
ATOM	1679	HD11	LEU	102	-1 943	1.395	8 316	1 00	0 00
ATOM	1680	HD12	LEU	102	-2 958	0 338	7 332	1 00	0 00
ATOM	1681	HD13	LEU	102	-3 549	1.928	7 818	1 00	0 00
ATOM	1682	CD2	LEU	102	-0 559	1.903	6 290	1 00	0 00
ATOM	1683	HD21	LEU	102	-0 147	2 788	5 827	1.00	0 00
ATOM	1684	HD22	LEU	102	-0 224	1 027	5 749	1.00	0 00
ATOM	1685	HD23	LEU	102	-0 220	1 841	7 313	1 00	0 00
ATOM	1686	C	LEU	102	-0 897	5.265	6 139	1 00	0 00
ATOM	1687	O	LEU	102	0 301	4 991	6 137	1 00	0 00
ATOM	1688	N	GLU	103	-1 414	6.266	5 433	1.00	0 00
ATOM	1689	HN	GLU	103	-2.377	6 439	5 484	1 00	0 00
ATOM	1690	CA	GLU	103	-0 581	7 132	4 612	1 00	0 00
ATOM	1691	HA	GLU	103	-0 056	6.514	3 900	1 00	0 00
ATOM	1692	CB	GLU	103	-1 446	8 146	3 857	1 00	0 00
ATOM	1693	HB1	GLU	103	-1 912	8 808	4 572	1.00	0 00
ATOM	1694	HB2	GLU	103	-2 220	7 612	3 320	1 00	0 00
ATOM	1695	CG	GLU	103	-0.670	8 991	2 860	1 00	0 00
ATOM	1696	HG1	GLU	103	-1 083	8 832	1 874	1 00	0 00
ATOM	1697	HG2	GLU	103	0 364	8 680	2 871	1 00	0.00
ATOM	1698	CD	GLU	103	-0 734	10.472	3 178	1 00	0 00
ATOM	1699	OE1	GLU	103	-1 856	10 996	3 342	1 00	0 00
ATOM	1700	OE2	GLU	103	0 337	11.108	3 264	1 00	0.00
ATOM	1701	C	GLU	103	0 439	7.858	5 478	1 00	0 00
ATOM	1702	O	GLU	103	1.644	7 658	5 334	1 00	0 00
ATOM	1703	N	LYS	104	-0 052	8 675	6 405	1 00	0 00
ATOM	1704	HN	LYS	104	-1 024	8 786	6 480	1 00	0 00
ATOM	1705	CA	LYS	104	0 821	9 417	7.306	1 00	0 00
ATOM	1706	HA	LYS	104	1 329	10 172	6 725	1 00	0 00
ATOM	1707	CB	LYS	104	-0.003	10 100	8 399	1 00	0 00
ATOM	1708	HB1	LYS	104	-0.949	9 589	8.492	1 00	0 00
ATOM	1709	HB2	LYS	104	0 530	10 024	9 335	1 00	0 00
ATOM	1710	CG	LYS	104	-0 278	11 569	8 125	1 00	0 00
ATOM	1711	HG1	LYS	104	0 635	12 128	8 261	1 00	0 00
ATOM	1712	HG2	LYS	104	-1 026	11.920	8.820	1 00	0 00
ATOM	1713	CD	LYS	104	-0 782	11 786	6 708	1 00	0 00
ATOM	1714	HD1	LYS	104	-0 960	10 824	6.248	1 00	0 00
ATOM	1715	HD2	LYS	104	-0 031	12 322	6 147	1 00	0.00
ATOM	1716	CE	LYS	104	-2 073	12 589	6 695	1 00	0 00
ATOM	1717	HE1	LYS	104	-2 601	12 384	5 775	1 00	0 00
ATOM	1718	HE2	LYS	104	-2 680	12 283	7 534	1 00	0 00
ATOM	1719	NZ	LYS	104	-1.817	14 053	6 791	1 00	0.00
ATOM	1720	HZ1	LYS	104	-2 239	14 433	7 661	1.00	0.00
ATOM	1721	HZ2	LYS	104	-2 233	14.543	5 973	1 00	0 00
ATOM	1722	HZ3	LYS	104	-0 793	14 236	6 806	1 00	0 00
ATOM	1723	C	LYS	104	1 860	8.497	7 941	1 00	0 00
ATOM	1724	O	LYS	104	2.995	8 903	8 184	1 00	0.00
ATOM	1725	N	PHE	105	1 460	7 259	8 213	1 00	0 00
ATOM	1726	HN	PHE	105	0 540	6 997	7 997	1 00	0 00
ATOM	1727	CA	PHE	105	2.351	6 279	8 824	1 00	0 00
ATOM	1728	HA	PHE	105	2 951	6.790	9 562	1 00	0 00
ATOM	1729	CB	PHE	105	1 536	5 184	9 515	1 00	0 00
ATOM	1730	HB1	PHE	105	2 007	4 228	9.338	1 00	0 00
ATOM	1731	HB2	PHE	105	0 540	5.171	9 097	1 00	0 00
ATOM	1732	CG	PHE	105	1 411	5 369	11 001	1.00	0 00
ATOM	1733	CD1	PHE	105	0 521	6 294	11 524	1 00	0 00
ATOM	1734	HD1	PHE	105	-0 083	6 887	10.853	1 00	0 00
ATOM	1735	CD2	PHE	105	2 177	4 614	11 874	1 00	0 00
ATOM	1736	HD2	PHE	105	2 872	3.889	11 478	1 00	0 00
ATOM	1737	CE1	PHE	105	0 400	6 465	12 890	1.00	0.00
ATOM	1738	HE1	PHE	105	-0 296	7 190	13.285	1 00	0.00
ATOM	1739	CE2	PHE	105	2 061	4 780	13.241	1 00	0.00
ATOM	1740	HE2	PHE	105	2 665	4.186	13 911	1 00	0 00
ATOM	1741	CZ	PHE	105	1.172	5 707	13 750	1 00	0 00
ATOM	1742	HZ	PHE	105	1 079	5 838	14 818	1.00	0 00
ATOM	1743	C	PHE	105	3 279	5 655	7 785	1 00	0.00
ATOM	1744	O	PHE	105	4 491	5 871	7 808	1 00	0.00
ATOM	1745	N	PHE	106	2.702	4 870	6 882	1 00	0 00
ATOM	1746	HN	PHE	106	1 732	4 732	6 922	1 00	0 00
ATOM	1747	CA	PHE	106	3 470	4 199	5 841	1 00	0 00
ATOM	1748	HA	PHE	106	4.078	3 441	6 316	1 00	0 00
ATOM	1749	CB	PHE	106	2 532	3 526	4 839	1 00	0 00
ATOM	1750	HB1	PHE	106	1 881	2 844	5.366	1.00	0 00
ATOM	1751	HB2	PHE	106	1 937	4 281	4.351	1 00	0 00
ATOM	1752	CG	PHE	106	3 254	2 755	3 777	1.00	0 00
ATOM	1753	CD1	PHE	106	3 931	1 590	4.091	1 00	0 00
ATOM	1754	HD1	PHE	106	3.928	1.235	5 109	1 00	0 00
ATOM	1755	CD2	PHE	106	3 267	3 202	2 469	1.00	0 00
ATOM	1756	HD2	PHE	106	2 743	4 111	2 214	1 00	0 00
ATOM	1757	CE1	PHE	106	4.601	0.879	3 118	1 00	0 00
ATOM	1758	HE1	PHE	106	5 122	-0.029	3 376	1 00	0.00
ATOM	1759	CE2	PHE	106	3.941	2.500	1.491	1.00	0.00
ATOM	1760	HE2	PHE	106	3.935	2.853	0.471	1.00	0.00
ATOM	1761	CZ	PHE	106	4 605	1.334	1 814	1 00	0 00
ATOM	1762	HZ	PHE	106	5.125	0 780	1 050	1.00	0.00
ATOM	1763	C	PHE	106	4 388	5 173	5 110	1 00	0.00
ATOM	1764	O	PHE	106	5 610	5.033	5 148	1 00	0 00
ATOM	1765	N	PHE	107	3 795	6.155	4 434	1 00	0 00
ATOM	1766	HN	PHE	107	2.814	6.212	4 432	1 00	0 00
ATOM	1767	CA	PHE	107	4 575	7 140	3 686	1 00	0 00
ATOM	1768	HA	PHE	107	5 076	6 616	2 885	1 00	0 00
ATOM	1769	CB	PHE	107	3 662	8 212	3 077	1 00	0 00
ATOM	1770	HB1	PHE	107	2 932	8.510	3 811	1 00	0 00
ATOM	1771	HB2	PHE	107	4 263	9 070	2 810	1 00	0 00
ATOM	1772	CG	PHE	107	2 918	7.770	1.838	1 00	0 00
ATOM	1773	CD1	PHE	107	3 038	6 475	1 348	1 00	0 00
ATOM	1774	HD1	PHE	107	3 674	5 771	1 863	1.00	0 00
ATOM	1775	CD2	PHE	107	2 098	8 660	1 160	1 00	0 00
ATOM	1776	HD2	PHE	107	1 995	9 670	1 528	1 00	0 00
ATOM	1777	CE1	PHE	107	2 356	6 080	0 214	1 00	0 00
ATOM	1778	HE1	PHE	107	2 460	5 069	-0 154	1 00	0 00
ATOM	1779	CE2	PHE	107	1 413	8.268	0 025	1 00	0 00
ATOM	1780	HE2	PHE	107	0 777	8 972	-0 492	1 00	0 00
ATOM	1781	CZ	PHE	107	1 542	6 977	-0 449	1 00	0 00
ATOM	1782	HZ	PHE	107	1.007	6 669	-1 336	1 00	0 00
ATOM	1783	C	PHE	107	5 636	7.787	4 571	1 00	0 00
ATOM	1784	O	PHE	107	6 638	8 301	4 075	1 00	0 00
ATOM	1785	N	SER	108	5 411	7.766	5 883	1 00	0 00
ATOM	1786	HN	SER	108	4 619	7 305	6 227	1 00	0 00
ATOM	1787	CA	SER	108	6 391	8 287	6 826	1 00	0 00
ATOM	1788	HA	SER	108	6 835	9 173	6 400	1 00	0 00
ATOM	1789	CB	SER	108	5 730	8 643	8 157	1 00	0 00
ATOM	1790	HB1	SER	108	6 468	8 597	8 942	1 00	0 00
ATOM	1791	HB2	SER	108	4 940	7.938	8 364	1.00	0 00
ATOM	1792	OG	SER	108	5 181	9 949	8 121	1 00	0 00
ATOM	1793	HG	SER	108	4.501	9 993	7 445	1 00	0 00
ATOM	1794	C	SER	108	7 471	7 243	7 042	1 00	0 00
ATOM	1795	O	SER	108	8 647	7 561	7.216	1 00	0.00
ATOM	1796	N	LYS	109	7 049	5 986	6.994	1 00	0 00
ATOM	1797	HN	LYS	109	6.100	5.811	6 828	1 00	0 00
ATOM	1798	CA	LYS	109	7 953	4 860	7 124	1 00	0 00
ATOM	1799	HA	LYS	109	8 620	5 053	7 951	1 00	0 00
ATOM	1800	CB	LYS	109	7 149	3.591	7 401	1 00	0 00
ATOM	1801	HB1	LYS	109	6 255	3 607	6 795	1 00	0 00
ATOM	1802	HB2	LYS	109	7 741	2 737	7 126	1 00	0 00
ATOM	1803	CG	LYS	109	6 734	3 440	8 856	1 00	0 00
ATOM	1804	HG1	LYS	109	5 820	2 866	8 902	1 00	0 00
ATOM	1805	HG2	LYS	109	6 566	4.421	9.276	1 00	0 00
ATOM	1806	CD	LYS	109	7 802	2 732	9 670	1.00	0 00
ATOM	1807	HD1	LYS	109	8 751	3.219	9 500	1 00	0 00
ATOM	1808	HD2	LYS	109	7.544	2 794	10 717	1 00	0 00
ATOM	1809	CE	LYS	109	7 919	1 269	9.276	1 00	0 00
ATOM	1810	HE1	LYS	109	6 930	0 835	9 254	1 00	0 00
ATOM	1811	HE2	LYS	109	8.359	1.209	8 292	1 00	0 00
ATOM	1812	NZ	LYS	109	8 763	0.502	10 233	1.00	0 00
ATOM	1813	HZ1	LYS	109	8 800	-0 499	9 955	1 00	0 00
ATOM	1814	HZ2	LYS	109	8 368	0 570	11.192	1 00	0 00
ATOM	1815	HZ3	LYS	109	9 731	0 883	10 241	1 00	0.00
ATOM	1816	C	LYS	109	8 769	4 700	5.846	1 00	0 00
ATOM	1817	O	LYS	109	9 948	4 348	5.882	1 00	0 00
ATOM	1818	N	ILE	110	8 127	4 989	4 717	1 00	0.00
ATOM	1819	HN	ILE	110	7 193	5.283	4.765	1.00	0 00
ATOM	1820	CA	ILE	110	8 780	4 928	3 416	1 00	0 00
ATOM	1821	HA	ILE	110	8 993	3.891	3 187	1 00	0.00
ATOM	1822	CB	ILE	110	7.850	5 488	2.313	1 00	0 00
ATOM	1823	HB	ILE	110	7.508	6 464	2.626	1 00	0 00
ATOM	1824	CG1	ILE	110	6 640	4 570	2 129	1 00	0 00
ATOM	1825	HG11	ILE	110	5 898	5.077	1 532	1 00	0 00
ATOM	1826	HG12	ILE	110	6 221	4.342	3 093	1 00	0 00
ATOM	1827	CG2	ILE	110	8.593	5 651	0.996	1 00	0.00
ATOM	1828	HG21	ILE	110	8 729	6 702	0.786	1 00	0 00
ATOM	1829	HG22	ILE	110	8 022	5 196	0 201	1 00	0 00
ATOM	1830	HG23	ILE	110	9 556	5 169	1.070	1 00	0.00
ATOM	1831	CD1	ILE	110	6 973	3 260	1 449	1 00	0 00
ATOM	1832	HD11	ILE	110	6 748	2.442	2 117	1 00	0 00
ATOM	1833	HD12	ILE	110	8 023	3 242	1 201	1 00	0 00
ATOM	1834	HD13	ILE	110	6 388	3.162	0 548	1.00	0.00
ATOM	1835	C	ILE	110	10 088	5 717	3 438	1 00	0.00
ATOM	1836	O	ILE	110	11 129	5 225	3 008	1 00	0.00
ATOM	1837	N	LYS	111	10 018	6 946	3 946	1 00	0 00
ATOM	1838	HN	LYS	111	9 153	7 278	4 263	1 00	0 00
ATOM	1839	CA	LYS	111	11 184	7 828	4 017	1 00	0 00
ATOM	1840	HA	LYS	111	11 336	8 250	3.035	1 00	0 00
ATOM	1841	CB	LYS	111	10 921	8 963	5.009	1.00	0 00
ATOM	1842	HB1	LYS	111	11 572	8 840	5 861	1 00	0 00
ATOM	1843	HB2	LYS	111	9 894	8 907	5 340	1 00	0 00
ATOM	1844	CG	LYS	111	11 156	10.346	4 425	1 00	0 00
ATOM	1845	HG1	LYS	111	11 692	10 245	3 493	1 00	0 00
ATOM	1846	HG2	LYS	111	11 746	10 925	5 121	1 00	0 00
ATOM	1847	CD	LYS	111	9 847	11 073	4 164	1 00	0 00
ATOM	1848	HD1	LYS	111	10 065	12.076	3.827	1 00	0.00
ATOM	1849	HD2	LYS	111	9 280	11 114	5 083	1 00	0.00
ATOM	1850	CE	LYS	111	9 018	10 367	3 104	1 00	0 00
ATOM	1851	HE1	LYS	111	8 683	9 419	3.499	1.00	0 00
ATOM	1852	HE2	LYS	111	9 636	10 195	2 235	1 00	0 00
ATOM	1853	NZ	LYS	111	7.830	11.169	2.702	1.00	0.00
ATOM	1854	HZ1	LYS	111	7.360	11.560	3.543	1.00	0.00
ATOM	1855	HZ2	LYS	111	7.151	10 571	2 187	1 00	0 00
ATOM	1856	HZ3	LYS	111	8 121	11 954	2.084	1 00	0 00
ATOM	1857	C	LYS	111	12 448	7 070	4 425	1 00	0.00
ATOM	1858	O	LYS	111	13 491	7 199	3.785	1 00	0 00
ATOM	1859	N	GLU	112	12 347	6 285	5 491	1 00	0 00
ATOM	1860	HN	GLU	112	11 489	6 225	5 962	1 00	0 00
ATOM	1861	CA	GLU	112	13 485	5 516	5 983	1 00	0.00
ATOM	1862	HA	GLU	112	14 297	6 205	6 161	1 00	0 00
ATOM	1863	CB	GLU	112	13.126	4 819	7.296	1 00	0 00
ATOM	1864	HB1	GLU	112	12.159	4 350	7 189	1 00	0.00
ATOM	1865	HB2	GLU	112	13 864	4 058	7 500	1 00	0 00
ATOM	1866	CG	GLU	112	13 070	5.760	8 489	1 00	0.00
ATOM	1867	HG1	GLU	112	12 440	5 320	9 249	1 00	0.00
ATOM	1868	HG2	GLU	112	12 644	6 700	8 169	1 00	0 00
ATOM	1869	CD	GLU	112	14 437	6 026	9 087	1 00	0 00
ATOM	1870	OE1	GLU	112	14 842	5 277	10 001	1 00	0 00
ATOM	1871	OE2	GLU	112	15 103	6.984	8 641	1 00	0 00
ATOM	1872	C	GLU	112	13 934	4 484	4.954	1 00	0 00
ATOM	1873	O	GLU	112	15 128	4.228	4 798	1 00	0 00
ATOM	1874	N	ALA	113	12.970	3 892	4 257	1 00	0 00
ATOM	1875	HN	ALA	113	12.037	4 138	4 430	1 00	0 00
ATOM	1876	CA	ALA	113	13.263	2 883	3 245	1 00	0 00
ATOM	1877	HA	ALA	113	14 151	2 356	3 550	1 00	0 00
ATOM	1878	CB	ALA	113	12 128	1 872	3 167	1 00	0.00
ATOM	1879	HB1	ALA	113	11.209	2 380	2.915	1 00	0.00
ATOM	1880	HB2	ALA	113	12 018	1.381	4.123	1 00	0 00
ATOM	1881	HB3	ALA	113	12 353	1 136	2.409	1 00	0 00
ATOM	1882	C	ALA	113	13 513	3 512	1 873	1.00	0 00
ATOM	1883	O	ALA	113	13 917	2 823	0 936	1 00	0 00
ATOM	1884	N	GLY	114	13 276	4 818	1.753	1 00	0 00
ATOM	1885	HN	GLY	114	12 946	5 324	2 523	1 00	0 00
ATOM	1886	CA	GLY	114	13.468	5 488	0 480	1 00	0.00
ATOM	1887	HA1	GLY	114	14 518	5 464	0 226	1 00	0 00
ATOM	1888	HA2	GLY	114	13 152	6 516	0.573	1.00	0 00
ATOM	1889	C	GLY	114	12 679	4 830	-0 634	1 00	0 00
ATOM	1890	O	GLY	114	13 227	4 056	-1.417	1 00	0 00
ATOM	1891	N	LEU	115	11 383	5 123	-0.690	1 00	0 00
ATOM	1892	HN	LEU	115	11.006	5 743	-0 033	1 00	0 00
ATOM	1893	CA	LEU	115	10 508	4 534	-1 697	1.00	0 00
ATOM	1894	HA	LEU	115	11 123	4 180	-2 510	1.00	0 00
ATOM	1895	CB	LEU	115	9.724	3 363	-1 104	1.00	0 00
ATOM	1896	HB1	LEU	115	9 340	3 668	-0 144	1 00	0 00
ATOM	1897	HB2	LEU	115	8 890	3 167	-1.754	1 00	0 00
ATOM	1898	CG	LEU	115	10 497	2 058	-0 907	1 00	0 00
ATOM	1899	HG	LEU	115	9 793	1 246	-0 833	1 00	0 00
ATOM	1900	CD1	LEU	115	11 280	2 102	0 391	1 00	0 00
ATOM	1901	HD11	LFU	115	10 719	1 597	1 166	1.00	0 00
ATOM	1902	HD12	LEU	115	11 440	3.130	0 676	1.00	0 00
ATOM	1903	HD13	LEU	115	12.231	1 611	0 255	1.00	0 00
ATOM	1904	CD2	LEU	115	11 414	1 774	-2 087	1 00	0.00
ATOM	1905	HD21	LEU	115	11 066	2.313	-2 953	1 00	0 00
ATOM	1906	HD22	LEU	115	11 409	0 715	-2.298	1 00	0 00
ATOM	1907	HD23	LEU	115	12 418	2 086	-1 846	1 00	0.00
ATOM	1908	C	LEU	115	9 509	5 550	-2 237	1 00	0 00
ATOM	1909	O	LEU	115	9 388	6 653	-1 709	1.00	0 00
ATOM	1910	N	ILE	116	8 752	5 124	-3 252	1.00	0 00
ATOM	1911	HN	ILE	116	8 896	4 217	-3 594	1 00	0 00
ATOM	1912	CA	ILE	116	7 707	5 945	-3 865	1.00	0 00
ATOM	1913	HA	ILE	116	7 395	5 441	-4.768	1 00	0 00
ATOM	1914	CB	ILE	116	6 469	6.061	-2 949	1 00	0 00
ATOM	1915	HB	ILE	116	6 730	6 669	-2 097	1 00	0.00
ATOM	1916	CG1	ILE	116	6 037	4 676	-2.458	1 00	0.00
ATOM	1917	HG11	ILE	116	5 298	4 265	-3 135	1 00	0.00
ATOM	1918	HG12	ILE	116	6 898	4 026	-2.435	1 00	0 00
ATOM	1919	CG2	ILE	116	5 326	6.743	-3.681	1 00	0 00
ATOM	1920	HG21	ILE	116	5 006	7 609	-3 121	1.00	0 00
ATOM	1921	HG22	ILE	116	4.502	6 052	-3 779	1.00	0 00
ATOM	1922	HG23	ILE	116	5 659	7.050	-4 661	1 00	0 00
ATOM	1923	CD1	ILE	116	5 433	4 694	-1 073	1 00	0 00
ATOM	1924	HD11	ILE	116	6 172	5 032	-0.363	1 00	0.00
ATOM	1925	HD12	ILE	116	5.110	3 698	-0 809	1.00	0 00
ATOM	1926	HD13	ILE	116	4.586	5 363	-1 057	1 00	0 00
ATOM	1927	C	ILE	116	8.213	7 340	-4 246	1.00	0 00
ATOM	1928	O	ILE	116	8 498	7.601	-5 415	1 00	0 00
ATOM	1929	N	ASP	117	8.305	8.240	-3 268	1 00	0 00
ATOM	1930	HN	ASP	117	8.072	7 979	-2 355	1.00	0 00
ATOM	1931	CA	ASP	117	8 776	9.600	-3 515	1 00	0.00
ATOM	1932	HA	ASP	117	8.982	10 054	-2.558	1 00	0 00
ATOM	1933	CB	ASP	117	10 063	9.583	-4 345	1 00	0 00
ATOM	1934	HB1	ASP	117	9 902	10 133	-5 260	1 00	0 00
ATOM	1935	HB2	ASP	117	10 317	8 560	-4 583	1.00	0.00
ATOM	1936	CG	ASP	117	11.233	10 208	-3 610	1 00	0 00
ATOM	1937	OD1	ASP	117	11.577	11 368	-3 920	1 00	0 00
ATOM	1938	OD2	ASP	117	11.804	9.538	-2 724	1 00	0 00
ATOM	1939	C	ASP	117	7.708	10.424	-4 226	1.00	0 00
ATOM	1940	O	ASP	117	8.020	11 293	-5 041	1 00	0 00
ATOM	1941	N	LYS	118	6.448	10 150	-3.906	1 00	0 00
ATOM	1942	HN	LYS	118	6 264	9 447	-3 247	1.00	0 00
ATOM	1943	CA	LYS	118	5 332	10 869	-4.508	1 00	0 00
ATOM	1944	HA	LYS	118	5 635	11.184	-5 496	1 00	0 00
ATOM	1945	CB	LYS	118	4 114	9 952	-4.628	1 00	0.00
ATOM	1946	HB1	LYS	118	3 696	9 798	-3 644	1 00	0 00

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ATOM   1947  HB2 LYS   118       4.432   9.001  -5.028  1.00  0.00
ATOM   1948  CG  LYS   118       3.021  10.506  -5.527  1.00  0.00
ATOM   1949  HG1 LYS   118       3.175  10.140  -6.531  1.00  0.00
ATOM   1950  HG2 LYS   118       3 077  11 585  -5 522  1.00  0 00
ATOM   1951  CD  LYS   118       1 642  10 081  -5 053  1 00  0 00
ATOM   1952  HD1 LYS   118       1.422   9 100  -5 449  1 00  0 00
ATOM   1953  HD2 LYS   118       1 637  10 044  -3.974  1.00  0 00
ATOM   1954  CE  LYS   118       0 569  11 052  -5 518  1 00  0 00
ATOM   1955  HE1 LYS   118      -0.025  11 347  -4 666  1.00  0.00
ATOM   1956  HE2 LYS   118       1.048  11 922  -5.942  1 00  0 00
ATOM   1957  NZ  LYS   118      -0.324  10 443  -6.543  1 00  0.00
ATOM   1958  HZ1 LYS   118      -0 734   9 558  -6 180  1 00  0 00
ATOM   1959  HZ2 LYS   118       0 214  10.234  -7 408  1 00  0 00
ATOM   1960  HZ3 LYS   118      -1 097  11 099  -6 778  1 00  0 00
ATOM   1961  C   LYS   118       4 974  12 103  -3 687  1 00  0 00
ATOM   1962  OT1 LYS   118       4.769  13 177  -4.291  1 00  0 00
ATOM   1963  OT2 LYS   118       4 901  11 986  -2 445  1 00  0 00
END
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Table 6

Atomic Structure Coordinates of the P/CAF Bromodomain/Acetyl-Histamine Complex

```
REMARK
FILENAME="/bloch2/chris/COMPLEX_XPLOR_ARIA7/structures/it8/complex_83 "REMARK
initial random number seed  5 960359E+10REMARK
=====================================================================REMARK
overall,bonds,angles,improper,vdw,noe,cdihREMARK energies  154 107, 9 85626,
72 1621, 0, 22.2303, 36 0151, 0 204524REMARK
=====================================================================REMARK
bonds,angles,impropers,noe,cdihREMARK rms-dev.  2 214961E-
03,0.361077,52 7899,1 40651E-02,0 249335REMARK
=====================================================================REMARK
noe,  cdihREMARK violations.  2, 0REMARK
=====================================================================REMARK DATE 05-
Dec-98  15 11.47       created by user ATOM      1  CA  ACE   200     -14 038
2 661   -4 705  1 00  0 00     AcH ATOM     2  HA1 ACE   200    -14.803
1 912   -4 558  1 00  0.00     AcH ATOM     3  HA2 ACE   200    -13 320
2 304   -5 428  1 00  0 00     AcH ATOM     4  HA3 ACE   200    -14 491
3 572   -5.067  1.00  0 00     AcH ATOM     5  C   ACE   200    -13 332
2 936   -3 376  1 00  0 00     AcH ATOM     6  O   ACE   200    -12.385
2 238   -3.012  1 00  0 00     AcH ATOM     7  N   HIM   201    -13.773
3 967   -2.663  1 00  0 00     AcH ATOM     8  HN  HIM   201    -13 586
4.875   -2.982  1.00  0 00     AcH ATOM     9  CA  HIM   201    -14 521
3 827   -1.417  1 00  0 00     AcH ATOM    10  HA1 HIM   201    -13 833
3 589   -0 620  1.00  0 00     AcH ATOM    11  HA2 HIM   201    -15 236
3 025   -1.526  1 00  0.00     AcH ATOM    12  CB  HIM   201    -15 268
5 100   -1 055  1.00  0 00     AcH ATOM    13  HB1 HIM   201    -14 591
5 940   -1 107  1 00  0 00     AcH ATOM    14  HB2 HIM   201    -15.669
5 009   -0 056  1 00  0 00     AcH ATOM    15  CG  HIM   201    -16.397
5 329   -2 010  1 00  0 00     AcH ATOM    16  ND1 HIM   201    -17 392
6 259   -1 793  1 00  0 00     AcH ATOM    17  HD1 HIM   201    -17 421
6 906   -1 057  1 00  0 00     AcH ATOM    18  CD2 HIM   201    -16 680
4 756   -3.204  1 00  0.00     AcH ATOM    19  HD2 HIM   201    -16 026
4 116   -3 779  1 00  0.00     AcH ATOM    20  CE1 HIM   201    -18 316
6 135   -2.729  1.00  0 00     AcH ATOM    21  HE1 HIM   201    -19 220
6 722   -2.806  1.00  0 00     AcH ATOM    22  NE2 HIM   201    -17 912
5 221   -3.592  1 00  0 00     AcH ATOM    23  CA  GLY     1     27 272
16 667   -0 366  1 00  0 00     BrD ATOM    24  HA1 GLY     1     28 103
16.198   -0 871  1.00  0 00     BrD ATOM    25  HA2 GLY     1     26 478
15 945   -0 255  1.00  0 00     BrD ATOM    26  C   GLY     1     27 724
17 114    1 011  1 00  0 00     BrD ATOM    27  O   GLY     1     28 713
17 834    1 144  1.00  0 00     BrD ATOM    28  N   GLY     1     26 780
17.800   -1 198  1.00  0.00     BrD ATOM    29  HT1 GLY     1     25 769
17.963   -1.018  1.00  0.00     BrD ATOM    30  HT2 GLY     1     26 911
17 584   -2.207  1.00  0 00     BrD ATOM    31  HT3 GLY     1     27 307
18 667   -0 970  1 00  0 00     BrD ATOM    32  N   SER     2     26 999
16 682    2 037  1 00  0.00     BrD ATOM    33  HN  SER     2     26.222
16 110    1 866  1 00  0 00     BrD ATOM    34  CA  SER     2     27 328
17.043    3 411  1 00  0 00     BrD ATOM    35  HA  SER     2     28 283
17 546    3.401  1 00  0 00     BrD ATOM    36  CB  SER     2     26 269
17 992    3 975  1 00  0 00     BrD ATOM    37  HB1 SER     2     26 705
18 588    4.762  1.00  0 00     BrD ATOM    38  HB2 SER     2     25 448
17 414    4 374  1.00  0 00     BrD ATOM    39  OG  SER     2     25 771
18 857    2 969  1 00  0 00     BrD ATOM    40  HG  SER     2     26 478
19.429    2.660  1 00  0 00     BrD ATOM    41  C   SER     2     27.435
15 801    4.290  1 00  0.00     BrD ATOM    42  O   SER     2     26 900
14 744    3.956  1 00  0 00     BrD ATOM    43  N   HIS     3     28 131
15 936    5 415  1.00  0.00     BrD ATOM    44  HN  HIS     3     28 534
16.803    5.627  1 00  0.00     BrD ATOM    45  CA  HIS     3     28 308
14 824    6 342  1.00  0 00     BrD ATOM    46  HA  HIS     3     28 652
13 972    5.775  1 00  0.00     BrD ATOM    47  CB  HIS     3     29 356
15 176    7 399  1 00  0 00     BrD ATOM    48  HB1 HIS     3     29 337
14 428    8.178  1 00  0 00     BrD ATOM    49  HB2 HIS     3     30 333
15.184    6.939  1.00  0 00     BrD ATOM    50  CG  HIS     3     29.137
16 512    8 039  1 00  0 00     BrD ATOM    51  ND1 HIS     3     28.235
16.718    9.062  1 00  0.00     BrD ATOM    52  HD1 HIS     3     27.659
16.035    9 465  1 00  0 00     BrD ATOM    53  CD2 HIS     3     29.710
17.715    7.796  1 00  0 00     BrD ATOM    54  HD2 HIS     3     30 468
17 927    7 055  1 00  0 00     BrD ATOM    55  CE1 HIS     3     28 262
17 991    9 420  1 00  0.00     BrD ATOM    56  HE1 HIS     3     27.661
18.442   10 196  1 00  0 00     BrD ATOM    57  NE2 HIS     3     29.148
18.615    8.668  1 00  0 00     BrD ATOM    58  HE2 HIS     3     29 368
19.568    8.725  1.00  0 00     BrD ATOM    59  C   HIS     3     26.991
14 463    7 020  1 00  0.00     BrD ATOM    60  O   HIS     3     26.660
14 998    8 078  1.00  0 00     BrD ATOM    61  N   MET     4     26.245
13 551    6 405  1.00  0.00     BrD ATOM    62  HN  MET     4     26 563
13.161    5 565  1 00  0 00     BrD ATOM    63  CA  MET     4     24.964
13.119    6 951  1.00  0.00     BrD ATOM    64  HA  MET     4     25 136
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12.767    7.958  1.00  0.00     BrD ATOM    65  CB  MET     4     23.985
14.294    6 994  1 00  0.00     BrD ATOM    66  HB1 MET     4     24.445
15.111    7 531  1.00  0 00     BrD ATOM    67  HB2 MET     4     23.776
14 612    5 984  1.00  0.00     BrD ATOM    68  CG  MET     4     22 665
13.962    7 672  1.00  0 00     BrD ATOM    69  HG1 MET     4     22 754
14 176    8.727  1.00  0.00     BrD ATOM    70  HG2 MET     4     22 461
12 911    7.535  1.00  0 00     BrD ATOM    71  SD  MET     4     21 283
14 909    7.006  1.00  0 00     BrD ATOM    72  CE  MET     4     22 027
16 531    6 842  1.00  0.00     BrD ATOM    73  HE1 MET     4     22 811
16.643    7.576  1.00  0.00     BrD ATOM    74  HE2 MET     4     21 274
17 289    7 000  1 00  0.00     BrD ATOM    75  HE3 MET     4     22.443
16.638    5 851  1 00  0 00     BrD ATOM    76  C   MET     4     24.376
11.977    6.126  1 00  0 00     BrD ATOM    77  O   MET     4     24 580
11.906    4 914  1.00  0 00     BrD ATOM    78  N   SER     5     23 650
11.084    6 792  1.00  0 00     BrD ATOM    79  HN  SER     5     23.528
11.194    7.758  1 00  0 00     BrD ATOM    80  CA  SER     5     23.040
9 939    6.125  1.00  0 00     BrD ATOM    81  HA  SER     5     23.836
9 303    5 767  1 00  0 00     BrD ATOM    82  CB  SER     5     22 177
9 148    7 111  1 00  0 00     BrD ATOM    83  HB1 SER     5     21 179
9 560    7 123  1 00  0 00     BrD ATOM    84  HB2 SER     5     22 136
8 114    6 801  1 00  0.00     BrD ATOM    85  OG  SER     5     22 712
9 210    8.421  1 00  0 00     BrD ATOM    86  HG  SER     5     23 243
8.428    8 588  1 00  0 00     BrD ATOM    87  C   SER     5     22 194
10 380    4 934  1.00  0.00     BrD ATOM    88  O   SER     5     21 748
11.525    4 867  1 00  0 00     BrD ATOM    89  N   LYS     6     21 973
9 460    3.999  1 00  0.00     BrD ATOM    90  HN  LYS     6     22 355
8 565    4.110  1.00  0 00     BrD ATOM    91  CA  LYS     6     21 180
9 753    2.811  1.00  0 00     BrD ATOM    92  HA  LYS     6     20.720
10 720    2 950  1.00  0 00     BrD ATOM    93  CB  LYS     6     22 078
9 801    1 572  1 00  0 00     BrD ATOM    94  HB1 LYS     6     21 474
10 056    0 714  1.00  0.00     BrD ATOM    95  HB2 LYS     6     22 512
8 824    1.418  1 00  0 00     BrD ATOM    96  CG  LYS     6     23 208
10 813    1 677  1 00  0 00     BrD ATOM    97  HG1 LYS     6     23 164
11 290    2.645  1.00  0.00     BrD ATOM    98  HG2 LYS     6     24 151
10 299    1 568  1 00  0 00     BrD ATOM    99  CD  LYS     6     23.100
11 879    0 598  1 00  0 00     BrD ATOM   100  HD1 LYS     6     22 401
11.546   -0 155  1.00  0.00     BrD ATOM   101  HD2 LYS     6     24.072
12.024    0.150  1 00  0 00     BrD ATOM   102  CE  LYS     6     22.618
13 203    1 168  1 00  0 00     BrD ATOM   103  HE1 LYS     6     21 595
13.088    1 494  1 00  0.00     BrD ATOM   104  HE2 LYS     6     22 666
13.953    0 393  1 00  0 00     BrD ATOM   105  NZ  LYS     6     23 448
13 645    2 322  1 00  0.00     BrD ATOM   106  HZ1 LYS     6     24 293
13.045    2 406  1 00  0 00     BrD ATOM   107  HZ2 LYS     6     22 900
13.578    3 204  1 00  0 00     BrD ATOM   108  HZ3 LYS     6     23 749
14.632    2 189  1 00  0 00     BrD ATOM   109  C   LYS     6     20 085
8 710    2.613  1 00  0 00     BrD ATOM   110  O   LYS     6     18 897
9.022    2.693  1 00  0 00     BrD ATOM   111  N   GLU     7     20.495
7 474    2.334  1 00  0 00     BrD ATOM   112  HN  GLU     7     21 457
7 295    2 280  1.00  0 00     BrD ATOM   113  CA  GLU     7     19 558
6 370    2 115  1 00  0 00     BrD ATOM   114  HA  GLU     7     20 083
5 603    1 565  1.00  0 00     BrD ATOM   115  CB  GLU     7     19.091
5 783    3 451  1 00  0.00     BrD ATOM   116  HB1 GLU     7     18 110
5 354    3 317  1 00  0 00     BrD ATOM   117  HB2 GLU     7     19 777
5 003    3 745  1 00  0 00     BrD ATOM   118  CG  GLU     7     19.014
6.799    4 579  1 00  0.00     BrD ATOM   119  HG1 GLU     7     18 377
7.614    4.271  1.00  0 00     BrD ATOM   120  HG2 GLU     7     20.007
7 173    4 780  1 00  0 00     BrD ATOM   121  CD  GLU     7     18 452
6 206    5.857  1 00  0 00     BrD ATOM   122  OE1 GLU     7     17 289
6 511    6.192  1 00  0 00     BrD ATOM   123  OE2 GLU     7     19.176
5 434    6.521  1.00  0 00     BrD ATOM   124  C   GLU     7     18.347
6 812    1.290  1 00  0 00     BrD ATOM   125  O   GLU     7     17 342
7 261    1 840  1.00  0 00     BrD ATOM   126  N   PRO     8     18 430
6 681   -0.045  1.00  0 00     BrD ATOM   127  CA  PRO     8     17 346
7 054   -0 951  1.00  0 00     BrD ATOM   128  HA  PRO     8     16 908
8 003   -0 677  1 00  0 00     BrD ATOM   129  CB  PRO     8     18.034
7 176   -2 321  1.00  0 00     BrD ATOM   130  HB1 PRO     8     17 603
6 458   -3 004  1.00  0 00     BrD ATOM   131  HB2 PRO     8     17.887
8 174   -2 708  1 00  0 00     BrD ATOM   132  CG  PRO     8     19 488
6 895   -2.087  1 00  0 00     BrD ATOM   133  HG1 PRO     8     19.876
6.286   -2 890  1 00  0.00     BrD ATOM   134  HG2 PRO     8     20 034
7 825   -2 026  1.00  0 00     BrD ATOM   135  CD  PRO     8     19 578
6 155   -0 784  1.00  0.00     BrD ATOM   136  HD1 PRO     8     20 504
6.384   -0 278  1 00  0 00     BrD ATOM   137  HD2 PRO     8     19 481
5.090   -0 943  1 00  0 00     BrD ATOM   138  C   PRO     8     16 259
5.987   -1 000  1.00  0.00     BrD ATOM   139  O   PRO     8     15 071
6.286   -0.874  1 00  0 00     BrD ATOM   140  N   ARG     9     16.680
4.740   -1.177  1.00  0 00     BrD ATOM   141  HN  ARG     9     17.640
4.570   -1 269  1 00  0 00     BrD ATOM   142  CA  ARG     9     15 754
3.617   -1.241  1 00  0 00     BrD ATOM   143  HA  ARG     9     15.272
3 529   -0.279  1.00  0.00     BrD ATOM   144  CB  ARG     9     14 692
3 864   -2.314  1 00  0 00     BrD ATOM   145  HB1 ARG     9     14.073
2 982   -2 402  1.00  0 00     BrD ATOM   146  HB2 ARG     9     14 076
4 696   -2 010  1.00  0.00     BrD ATOM   147  CG  ARG     9     15 272
4 176   -3 684  1 00  0.00     BrD ATOM   148  HG1 ARG     9     16.153
3.571   -3.837  1 00  0.00     BrD ATOM   149  HG2 ARG     9     15.539
5.221   -3 721  1 00  0 00     BrD ATOM   150  CD  ARG     9     14 274
3.882   -4 793  1.00  0.00     BrD ATOM   151  HD1 ARG     9     13.277
4.055   -4 417  1.00  0.00     BrD ATOM   152  HD2 ARG     9     14 375
2.848   -5.085  1.00  0 00     BrD ATOM   153  NE  ARG     9     14 493
4.728   -5.963  1.00  0 00     BrD ATOM   154  HE  ARG     9     14 761
4.289   -6.797  1 00  0.00     BrD ATOM   155  CZ  ARG     9     14.350
6.049   -5 955  1.00  0.00     BrD ATOM   156  NH1 ARG     9     13 988
6 672   -4 842  1 00  0.00     BrD ATOM   157 HH11 ARG     9     13.823
6 147   -4 006  1 00  0 00     BrD ATOM   158 HH12 ARG     9     13.880
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7.666   -4.837  1.00  0.00     BrD ATOM   159  NH2 ARG     9     14.567
6.749   -7.059  1 00  0.00     BrD ATOM   160 HH21 ARG     9     14.458
7.744   -7 051  1 00  0.00     BrD ATOM   161 HH22 ARG     9     14 840
6 284   -7.901  1.00  0.00     BrD ATOM   162  C   ARG     9     16.500
2 320   -1 538  1 00  0 00     BrD ATOM   163  O   ARG     9     17.367
2 278   -2 410  1.00  0 00     BrD ATOM   164  N   ASP    10     16 159
1 267   -0 803  1.00  0.00     BrD ATOM   165  HN  ASP    10     15 462
1 367   -0.123  1 00  0 00     BrD ATOM   166  CA  ASP    10     16 788  -
0 038   -0.988  1 00  0 00     BrD ATOM   167  HA  ASP    10     17.625
0 088   -1.658  1 00  0.00     BrD ATOM   168  CB  ASP    10     17 296  -
0 576    0 350  1 00  0.00     BrD ATOM   169  HB1 ASP    10     18.082
0.067    0 715  1.00  0.00     BrD ATOM   170  HB2 ASP    10     17.688  -
1 572    0 204  1.00  0 00     BrD ATOM   171  CG  ASP    10     16.203  -
0 641    1.399  1.00  0 00     BrD ATOM   172  OD1 ASP    10     16.210  -
1 595    2 205  1.00  0.00     BrD ATOM   173  OD2 ASP    10     15.340
0.262    1 413  1.00  0 00     BrD ATOM   174  C   ASP    10     15 803  -
1 028   -1 606  1 00  0 00     BrD ATOM   175  O   ASP    10     14 986  -
1 622   -0.903  1 00  0.00     BrD ATOM   176  N   PRO    11     15 866  -
1 218   -2.936  1 00  0.00     BrD ATOM   177  CA  PRO    11     14 974  -
2.118   -3 657  1 00  0.00     BrD ATOM   178  HA  PRO    11     13.975  -
2.098   -3.247  1 00  0 00     BrD ATOM   179  CB  PRO    11     14 958  -
1.540   -5.084  1.00  0 00     BrD ATOM   180  HB1 PRO    11     13.973  -
1 156   -5 302  1.00  0.00     BrD ATOM   181  HB2 PRO    11     15 203  -
2 321   -5 789  1 00  0 00     BrD ATOM   182  CG  PRO    11     15 982  -
0 443   -5.113  1.00  0 00     BrD ATOM   183  HG1 PRO    11     15 487
0 516   -5.149  1 00  0.00     BrD ATOM   184  HG2 PRO    11     16 620  -
0 564   -5.976  1 00  0.00     BrD ATOM   185  CD  PRO    11     16 792  -
0 558   -3 852  1 00  0 00     BrD ATOM   186  HD1 PRO    11     17.066
0.418   -3 487  1 00  0.00     BrD ATOM   187  HD2 PRO    11     17 671  -
1,163   -4.018  1 00  0.00     BrD ATOM   188  C   PRO    11     15.488  -
3 554   -3.670  1 00  0.00     BrD ATOM   189  O   PRO    11     15 551  -
4 191   -4.721  1 00  0.00     BrD ATOM   190  N   ASP    12     15 849  -
4 061   -2 496  1 00  0.00     BrD ATOM   191  HN  ASP    12     15 780  -
3 506   -1.691  1 00  0.00     BrD ATOM   192  CA  ASP    12     16 361  -
5 421   -2 384  1 00  0 00     BrD ATOM   193  HA  ASP    12     16 155  -
5 927   -3 315  1 00  0.00     BrD ATOM   194  CB  ASP    12     17 873  -
5 399   -2 151  1 00  0 00     BrD ATOM   195  HB1 ASP    12     18 123  -
6 112   -1 380  1.00  0 00     BrD ATOM   196  HB2 ASP    12     18 167  -
4 410   -1 830  1.00  0 00     BrD ATOM   197  CG  ASP    12     18.657  -
5 749   -3.400  1.00  0 00     BrD ATOM   198  OD1 ASP    12     18 450  -
5 084   -4.437  1 00  0.00     BrD ATOM   199  OD2 ASP    12     19.478  -
6 687   -3.342  1 00  0.00     BrD ATOM   200  C   ASP    12     15 674  -
6 179   -1.253  1.00  0.00     BrD ATOM   201  O   ASP    12     15 106  -
7 250   -1.468  1 00  0 00     BrD ATOM   202  N   GLN    13     15 740  -
5 626   -0 047  1 00  0.00     BrD ATOM   203  HN  GLN    13     16 206  -
4.770    0 063  1.00  0 00     BrD ATOM   204  CA  GLN    13     15 122  -
6 258    1 113  1 00  0.00     BrD ATOM   205  HA  GLN    13     15.336  -
7 316    1 069  1 00  0 00     BrD ATOM   206  CB  GLN    13     15.701  -
5 684    2 405  1.00  0 00     BrD ATOM   207  HB1 GLN    13     16.666  -
5 251    2 193  1.00  0 00     BrD ATOM   208  HB2 GLN    13     15 041  -
4 910    2.768  1 00  0.00     BrD ATOM   209  CG  GLN    13     15 870  -
6.719    3.505  1 00  0.00     BrD ATOM   210  HG1 GLN    13     15 520  -
6 297    4.436  1 00  0 00     BrD ATOM   211  HG2 GLN    13     15 277  -
7 587    3 258  1 00  0 00     BrD ATOM   212  CD  GLN    13     17.313  -
7 150    3.683  1 00  0.00     BrD ATOM   213  OE1 GLN    13     18 036  -
6 611    4 520  1.00  0.00     BrD ATOM   214  NE2 GLN    13     17 739  -
8 128    2 892  1.00  0 00     BrD ATOM   215 HE21 GLN    13     18 668  -
8.427    2 985  1 00  0 00     BrD ATOM   216 HE22 GLN    13     17 108  -
8 512    2 248  1 00  0 00     BrD ATOM   217  C   GLN    13     13 615  -
6.060    1 097  1.00  0.00     BrD ATOM   218  O   GLN    13     12 855  -
6 950    1.478  1.00  0 00     BrD ATOM   219  N   LEU    14     13.191  -
4.880    0 662  1.00  0 00     BrD ATOM   220  HN  LEU    14     13 848  -
4.214    0 371  1 00  0 00     BrD ATOM   221  CA  LEU    14     11 774  -
4 558    0 595  1.00  0.00     BrD ATOM   222  HA  LEU    14     11 303  -
4 943    1.487  1 00  0.00     BrD ATOM   223  CB  LEU    14     11.581  -
3 042    0 541  1 00  0.00     BrD ATOM   224  HB1 LEU    14     12 212  -
2.592    1.292  1 00  0.00     BrD ATOM   225  HB2 LEU    14     10.552  -
2.823    0 781  1 00  0.00     BrD ATOM   226  CG  LEU    14     11.905  -
2 399   -0 808  1 00  0 00     BrD ATOM   227  HG  LEU    14     12.685  -
2 967   -1 292  1 00  0.00     BrD ATOM   228  CD1 LEU    14     12 409  -
0 978   -0.615  1 00  0.00     BrD ATOM   229 HD11 LEU    14     11 569  -
0.311   -0.497  1 00  0.00     BrD ATOM   230 HD12 LEU    14     12 986  -
0 682   -1.479  1 00  0 00     BrD ATOM   231 HD13 LEU    14     13 032  -
0.934    0.266  1 00  0.00     BrD ATOM   232  CD2 LEU    14     10.682  -
2 418   -1.709  1.00  0.00     BrD ATOM   233 HD21 LEU    14     10 185  -
1 461   -1 660  1 00  0.00     BrD ATOM   234 HD22 LEU    14     10.005  -
3 192   -1 383  1 00  0.00     BrD ATOM   235 HD23 LEU    14     10 989  -
2 612   -2 727  1.00  0 00     BrD ATOM   236  C   LEU    14     11.130  -
5.209   -0 623  1 00  0 00     BrD ATOM   237  O   LEU    14      9.989  -
5.666   -0 564  1.00  0.00     BrD ATOM   238  N   TYR    15     11.866  -
5.241   -1 729  1.00  0.00     BrD ATOM   239  HN  TYR    15     12.772  -
4.865   -1.714  1 00  0.00     BrD ATOM   240  CA  TYR    15     11.364  -
5.841   -2.959  1 00  0.00     BrD ATOM   241  HA  TYR    15     10.539  -
5.237   -3.312  1 00  0 00     BrD ATOM   242  CB  TYR    15     12 460  -
5 865   -4.029  1.00  0 00     BrD ATOM   243  HB1 TYR    15     13 317  -
6 397   -3.642  1.00  0 00     BrD ATOM   244  HB2 TYR    15     12 748  -
4 850   -4.259  1.00  0.00     BrD ATOM   245  CG  TYR    15     12 043  -
6 533   -5 323  1.00  0.00     BrD ATOM   246  CD1 TYR    15     12 993  -
7.047   -6 197  1.00  0.00     BrD ATOM   247  HD1 TYR    15     14 040  -
6 968   -5 940  1.00  0 00     BrD ATOM   248  CD2 TYR    15     10.702  -
6.642   -5.675  1.00  0 00     BrD ATOM   249  HD2 TYR    15      9 950  -
6 248   -5 008  1.00  0.00     BrD ATOM   250  CE1 TYR    15     12.620  -
7.654   -7 381  1.00  0 00     BrD ATOM   251  HE1 TYR    15     13 374  -
8 049   -8.046  1 00  0 00     BrD ATOM   252  CE2 TYR    15     10.322  -
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7.249	-6.857	1.00	0.00	BrD ATOM	253	HE2	TYR	15	9.275 -
7.326	-7.111	1.00	0.00	BrD ATOM	254	CZ	TYR	15	11.284 -
7 752	-7 706	1 00	0 00	BrD ATOM	255	OH	TYR	15	10 908 -
8 358	-8 883	1 00	0 00	BrD ATOM	256	HH	TYR	15	10 572 -
9 238	-8 697	1 00	0 00	BrD ATOM	257	C	TYR	15	10 859 -
7 253	-2 696	1 00	0.00	BrD ATOM	258	O	TYR	15	9.778 -
7 630	-3 146	1 00	0 00	BrD ATOM	259	N	SER	16	11 641 -
8 026	-1 950	1 00	0 00	BrD ATOM	260	HN	SER	16	12 485 -
7 666	-1 605	1 00	0.00	BrD ATOM	261	CA	SER	16	11.249 -
9 384	-1 602	1 00	0 00	BrD ATOM	262	HA	SER	16	11 148 -
9 946	-2 518	1.00	0 00	BrD ATOM	263	CB	SER	16	12.315 -
10.040	-0 722	1 00	0.00	BrD ATOM	264	HB1	SER	16	12 503 -
9 416	0 139	1 00	0.00	BrD ATOM	265	HB2	SER	16	13.227 -
10 155	-1.289	1 00	0 00	BrD ATOM	266	OG	SER	16	11.892 -
11 317	-0 276	1 00	0 00	BrD ATOM	267	HG	SER	16	12 601 -
11 952	-0 405	1 00	0 00	BrD ATOM	268	C	SER	16	9 909 -
9 370	-0 879	1 00	0 00	BrD ATOM	269	O	SER	16	9 028 -
10 182	-1 161	1 00	0.00	BrD ATOM	270	N	THR	17	9 756 -
8 420	0 038	1 00	0 00	BrD ATOM	271	HN	THR	17	10 493 -
7 796	0 207	1 00	0 00	BrD ATOM	272	CA	THR	17	8 514 -
8 269	0 785	1 00	0 00	BrD ATOM	273	HA	THR	17	8 318 -
9 200	1 296	1 00	0 00	BrD ATOM	274	CB	THR	17	8 656 -
7 146	1 820	1 00	0 00	BrD ATOM	275	HB	THR	17	9 069 -
6 275	1 333	1 00	0 00	BrD ATOM	276	OG1	THR	17	9 539 -
7 535	2.857	1 00	0 00	BrD ATOM	277	HG1	THR	17	10 426 -
7 633	2 502	1 00	0 00	BrD ATOM	278	CG2	THR	17	7 346 -
6 733	2.463	1 00	0 00	BrD ATOM	279	HG21	THR	17	6 714 -
7 600	2 589	1 00	0 00	BrD ATOM	280	HG22	THR	17	6 845 -
6 012	1 832	1 00	0 00	BrD ATOM	281	HG23	THR	17	7 545 -
6 289	3 427	1 00	0 00	BrD ATOM	282	C	THR	17	7 356 -
7 971	-0 161	1 00	0 00	BrD ATOM	283	O	THR	17	6 420 -
8 757	-0 277	1 00	0 00	BrD ATOM	284	N	LEU	18	7.438 -
6 832	-0.843	1 00	0 00	BrD ATOM	285	HN	LEU	18	8.212 -
6 247	-0 702	1 00	0 00	BrD ATOM	286	CA	LEU	18	6.396 -
6.414	-1 776	1 00	0 00	BrD ATOM	287	HA	LEU	18	5.534 -
6.122	-1 197	1 00	0 00	BrD ATOM	288	CB	LEU	18	6.871 -
5 218	-2 591	1 00	0 00	BrD ATOM	289	HB1	LEU	18	7.669 -
5.542	-3 243	1 00	0 00	BrD ATOM	290	HB2	LEU	18	6 049 -
4 869	-3.198	1 00	0 00	BrD ATOM	291	CG	LEU	18	7.377 -
4.056	-1 750	1 00	0 00	BrD ATOM	292	HG	LEU	18	8 301 -
4 350	-1 275	1 00	0 00	BrD ATOM	293	CD1	LEU	18	7 653 -
2 840	-2 622	1.00	0 00	BrD ATOM	294	HD11	LEU	18	6 966 -
2 832	-3 455	1 00	0 00	BrD ATOM	295	HD12	LEU	18	8 667 -
2 885	-2 994	1.00	0 00	BrD ATOM	296	HD13	LEU	18	7 523 -
1 941	-2 039	1.00	0 00	BrD ATOM	297	CD2	LEU	18	6 369 -
3.727	-0 658	1 00	0 00	BrD ATOM	298	HD21	LEU	18	5 417 -
4.180	-0 897	1 00	0 00	BrD ATOM	299	HD22	LEU	18	6 252 -
2 657	-0 584	1 00	0 00	BrD ATOM	300	HD23	LEU	18	6 722 -
4 117	0 284	1 00	0 00	BrD ATOM	301	C	LEU	18	5 998 -
7 542	-2 707	1.00	0 00	BrD ATOM	302	O	LEU	18	4 869 -
8 021	-2 667	1.00	0 00	BrD ATOM	303	N	LYS	19	6 926 -
7.967	-3 552	1 00	0 00	BrD ATOM	304	HN	LYS	19	7.813 -
7 550	-3 543	1 00	0 00	BrD ATOM	305	CA	LYS	19	6 648 -
9.050	-4 487	1 00	0 00	BrD ATOM	306	HA	LYS	19	5 959 -
8 673	-5 228	1.00	0.00	BrD ATOM	307	CB	LYS	19	7 935 -
9 498	-5 193	1 00	0 00	BrD ATOM	308	HB1	LYS	19	7 671 -
9 974	-6 126	1 00	0 00	BrD ATOM	309	HB2	LYS	19	8 535 -
8 625	-5 404	1.00	0 00	BrD ATOM	310	CG	LYS	19	8 785 -
10 472	-4 390	1.00	0 00	BrD ATOM	311	HG1	LYS	19	8 296 -
11 438	-4 386	1 00	0 00	BrD ATOM	312	HG2	LYS	19	8 878 -
10 106	-3 378	1 00	0 00	BrD ATOM	313	CD	LYS	19	10 172 -
10 621	-4 992	1 00	0.00	BrD ATOM	314	HD1	LYS	19	10 575 -
9.638	-5 190	1 00	0 00	BrD ATOM	315	HD2	LYS	19	10 807 -
11 137	-4 287	1 00	0 00	BrD ATOM	316	CE	LYS	19	10 133 -
11 409	-6.290	1.00	0 00	BrD ATOM	317	HE1	LYS	19	9.337 -
11.019	-6 908	1 00	0 00	BrD ATOM	318	HE2	LYS	19	11 077 -
11 288	-6 800	1.00	0 00	BrD ATOM	319	NZ	LYS	19	9 893 -
12 858	-6.050	1 00	0.00	BrD ATOM	320	HZ1	LYS	19	9.982 -
13 072	-5 036	1.00	0 00	BrD ATOM	321	HZ2	LYS	19	10 587 -
13.427	-6 576	1.00	0 00	BrD ATOM	322	HZ3	LYS	19	8 937 -
13.119	-6 366	1 00	0 00	BrD ATOM	323	C	LYS	19	5 988 -
10.223	-3 761	1 00	0.00	BrD ATOM	324	O	LYS	19	5.193 -
10.960	-4 341	1 00	0 00	BrD ATOM	325	N	SER	20	6 299 -
10 359	-2.474	1 00	0 00	BrD ATOM	326	HN	SER	20	6 925 -
9.721	-2 061	1 00	0 00	BrD ATOM	327	CA	SER	20	5 722 -
11 425	-1 661	1 00	0 00	BrD ATOM	328	HA	SER	20	5 660 -
12.306	-2 277	1 00	0 00	BrD ATOM	329	CB	SER	20	6 608 -
11.725	-0 449	1 00	0 00	BrD ATOM	330	HB1	SER	20	7 086 -
10 815	-0 120	1 00	0 00	BrD ATOM	331	HB2	SER	20	5 999 -
12 121	0 350	1 00	0.00	BrD ATOM	332	OG	SER	20	7 610 -
12 674	-0 772	1 00	0.00	BrD ATOM	333	HG	SER	20	7 218 -
13.396	-1 269	1 00	0.00	BrD ATOM	334	C	SER	20	4.316 -
11 056	-1 207	1 00	0 00	BrD ATOM	335	O	SER	20	3 334 -
11 659	-1 642	1 00	0 00	BrD ATOM	336	N	ILE	21	4.218 -
10.045	-0 349	1.00	0 00	BrD ATOM	337	HN	ILE	21	5 031 -
9 592	-0 044	1 00	0 00	BrD ATOM	338	CA	ILE	21	2 919 -
9 583	0 129	1 00	0.00	BrD ATOM	339	HA	ILE	21	2.508 -
10 348	0 771	1 00	0 00	BrD ATOM	340	CB	ILE	21	3 036 -
8.280	0 945	1 00	0 00	BrD ATOM	341	HB	ILE	21	2 050 -
7.850	1 036	1 00	0 00	BrD ATOM	342	CG1	ILE	21	3.956 -
7.280	0 240	1.00	0 00	BrD ATOM	343	HG11	ILE	21	4 639 -
6.858	0 962	1 00	0.00	BrD ATOM	344	HG12	ILE	21	4 519 -
7 792	-0 521	1.00	0 00	BrD ATOM	345	CG2	ILE	21	3 549 -
8 579	2 346	1 00	0 00	BrD ATOM	346	HG21	ILE	21	4 618 -
8.431	2.377	1.00	0.00	BrD ATOM	347	HG22	ILE	21	3.319 -
9.603	2.603	1.00	0.00	BrD ATOM	348	HG23	ILE	21	3.073 -
7 915	3 053	1 00	0 00	BrD ATOM	349	CD1	ILE	21	3 222 -
6 140	-0 427	1 00	0.00	BrD ATOM	350	HD11	ILE	21	3 805 -
5 235	-0 338	1 00	0 00	BrD ATOM	351	HD12	ILE	21	2 264 -
6 000	0 051	1 00	0.00	BrD ATOM	352	HD13	ILE	21	3 075 -
6 371	-1 472	1 00	0.00	BrD ATOM	353	C	ILE	21	1.969 -
9.361	-1.044	1 00	0 00	BrD ATOM	354	O	ILE	21	0.869 -
9 901	-1.074	1 00	0.00	BrD ATOM	355	N	LEU	22	2 433 -
8 608	-2 034	1 00	0 00	BrD ATOM	356	HN	LEU	22	3.325 -
8 224	-1 957	1.00	0.00	BrD ATOM	357	CA	LEU	22	1 648 -
8.337	-3.229	1.00	0 00	BrD ATOM	358	HA	LEU	22	0 757 -
7 807	-2 929	1 00	0 00	BrD ATOM	359	CB	LEU	22	2 451 -
7 465	-4 197	1.00	0 00	BrD ATOM	360	HB1	LEU	22	3.352 -
7 996	-4 462	1.00	0.00	BrD ATOM	361	HB2	LEU	22	2 728 -
6.556	-3 683	1 00	0 00	BrD ATOM	362	CG	LEU	22	1 722 -
7 084	-5 486	1 00	0.00	BrD ATOM	363	HG	LEU	22	1 378 -
7 982	-5 977	1 00	0 00	BrD ATOM	364	CD1	LEU	22	2 665 -
6 362	-6 437	1 00	0 00	BrD ATOM	365	HD11	LEU	22	2 220 -
6 314	-7 419	1 00	0 00	BrD ATOM	366	HD12	LEU	22	3 601 -
6 898	-6 492	1 00	0 00	BrD ATOM	367	HD13	LEU	22	2.845 -
5 361	-6 074	1 00	0 00	BrD ATOM	368	CD2	LEU	22	0 507 -
6 222	-5 178	1 00	0 00	BrD ATOM	369	HD21	LEU	22	0 127 -
6 472	-4 199	1 00	0 00	BrD ATOM	370	HD22	LEU	22	-0 259 -
6 401	-5 918	1 00	0 00	BrD ATOM	371	HD23	LEU	22	0 790 -
5 180	-5 199	1 00	0 00	BrD ATOM	372	C	LEU	22	1 243 -
9 636	-3 915	1 00	0 00	BrD ATOM	373	O	LEU	22	0 086 -
9 813	-4 295	1.00	0 00	BrD ATOM	374	N	GLN	23	2 201 -
10 552	-4 058	1 00	0.00	BrD ATOM	375	HN	GLN	23	3 107 -
10 354	-3 735	1 00	0 00	BrD ATOM	376	CA	GLN	23	1.941 -
11 841	-4 693	1.00	0 00	BrD ATOM	377	HA	GLN	23	1.828 -
11 670	-5 754	1 00	0 00	BrD ATOM	378	CB	GLN	23	3 118 -
12 793	-4 464	1 00	0 00	BrD ATOM	379	HB1	GLN	23	3.720 -
12 412	-3 653	1 00	0 00	BrD ATOM	380	HB2	GLN	23	2 731 -
13 763	-4 186	1.00	0.00	BrD ATOM	381	CG	GLN	23	4.012 -
12 969	-5 682	1.00	0 00	BrD ATOM	382	HG1	GLN	23	4 318 -
11 995	-6 035	1.00	0 00	BrD ATOM	383	HG2	GLN	23	4.886 -
13 535	-5 393	1 00	0 00	BrD ATOM	384	CD	GLN	23	3 316 -
13 697	-6 815	1 00	0 00	BrD ATOM	385	OE1	GLN	23	2 624 -
14 692	-6 597	1 00	0 00	BrD ATOM	386	NE2	GLN	23	3 494 -
13 203	-8 034	1 00	0 00	BrD ATOM	387	HE21	GLN	23	4 058 -
12 408	-8 134	1 00	0 00	BrD ATOM	388	HE22	GLN	23	3 055 -
13 654	-8 786	1.00	0.00	BrD ATOM	389	C	GLN	23	0 655 -
12 467	-4 157	1 00	0.00	BrD ATOM	390	O	GLN	23	-0 207 -
12 892	-4 925	1 00	0.00	BrD ATOM	391	N	GLN	24	0 530 -
12 519	-2 833	1 00	0.00	BrD ATOM	392	HN	GLN	24	1 252 -
12 167	-2 269	1 00	0.00	BrD ATOM	393	CA	GLN	24	-0 654 -
13 096	-2.203	1 00	0 00	BrD ATOM	394	HA	GLN	24	-0 951 -
13.947	-2 797	1 00	0.00	BrD ATOM	395	CB	GLN	24	-0 325 -
13 584	-0 783	1 00	0 00	BrD ATOM	396	HB1	GLN	24	0 666 -
14 012	-0 785	1.00	0 00	BrD ATOM	397	HB2	GLN	24	-1 035 -
14.351	-0 509	1 00	0 00	BrD ATOM	398	CG	GLN	24	-0 369 -
12 498	0 284	1.00	0 00	BrD ATOM	399	HG1	GLN	24	-1 331 -
12 531	0 774	1.00	0 00	BrD ATOM	400	HG2	GLN	24	-0 243 -
11 539	-0 192	1.00	0 00	BrD ATOM	401	CD	GLN	24	0 714 -
12 663	1 333	1 00	0.00	BrD ATOM	402	OE1	GLN	24	0 426 -
12 791	2 524	1.00	0.00	BrD ATOM	403	NE2	GLN	24	1.967 -
12 659	0 897	1.00	0 00	BrD ATOM	404	HE21	GLN	24	2.122 -
12 552	-0 065	1.00	0.00	BrD ATOM	405	HE22	GLN	24	2 687 -
12.763	1 554	1.00	0.00	BrD ATOM	406	C	GLN	24	-1 816 -
12.099	-2.179	1 00	0.00	BrD ATOM	407	O	GLN	24	-2.974 -
12 485	-2 331	1.00	0.00	BrD ATOM	408	N	VAL	25	-1 501 -
10 821	-1.974	1 00	0.00	BrD ATOM	409	HN	VAL	25	-0 561 -
10.575	-1 859	1 00	0 00	BrD ATOM	410	CA	VAL	25	-2 523 -
9 776	-1 922	1 00	0 00	BrD ATOM	411	HA	VAL	25	-3 121 -
9 941	-1 036	1 00	0 00	BrD ATOM	412	CB	VAL	25	-1 890 -
8 369	-1 813	1 00	0 00	BrD ATOM	413	HB	VAL	25	-1 198 -
8 243	-2 632	1 00	0 00	BrD ATOM	414	CG1	VAL	25	-1 116 -
8 236	-0 510	1 00	0 00	BrD ATOM	415	HG11	VAL	25	-1 590 -
7 494	0 116	1.00	0 00	BrD ATOM	416	HG12	VAL	25	-0 102 -
7 932	-0 722	1.00	0 00	BrD ATOM	417	HG13	VAL	25	-1 108 -
9 186	0 003	1 00	0 00	BrD ATOM	418	CG2	VAL	25	-2 945 -
7 277	-1 908	1.00	0 00	BrD ATOM	419	HG21	VAL	25	-3 437 -
7 331	-2 868	1 00	0 00	BrD ATOM	420	HG22	VAL	25	-2 472 -
6 313	-1 799	1 00	0 00	BrD ATOM	421	HG23	VAL	25	-3 672 -
7.410	-1.121	1 00	0.00	BrD ATOM	422	C	VAL	25	-3.440 -
9 846	-3 141	1 00	0 00	BrD ATOM	423	O	VAL	25	-4.659 -
9 930	-3 000	1 00	0 00	BrD ATOM	424	N	LYS	26	-2 858 -
9 858	-4 336	1.00	0 00	BrD ATOM	425	HN	LYS	26	-1 883 -
9.798	-4 396	1 00	0 00	BrD ATOM	426	CA	LYS	26	-3.648 -
9.943	-5 562	1 00	0.00	BrD ATOM	427	HA	LYS	26	-4 174 -
9 008	-5.678	1.00	0 00	BrD ATOM	428	CB	LYS	26	-2 737 -
10 161	-6 771	1.00	0 00	BrD ATOM	429	HB1	LYS	26	-3 314 -
10 018	-7 673	1 00	0 00	BrD ATOM	430	HB2	LYS	26	-1.942 -
9 430	-6 744	1 00	0 00	BrD ATOM	431	CG	LYS	26	-2 111 -
11 545	-6 820	1 00	0 00	BrD ATOM	432	HG1	LYS	26	-2 070 -
11 947	-5 818	1 00	0 00	BrD ATOM	433	HG2	LYS	26	-2 721 -
12.183	-7 442	1 00	0.00	BrD ATOM	434	CD	LYS	26	-0 702 -
11 500	-7 391	1 00	0.00	BrD ATOM	435	HD1	LYS	26	-0.214 -
10.600	-7.048	1 00	0.00	BrD ATOM	436	HD2	LYS	26	-0.156 -
12.364	-7.043	1.00	0.00	BrD ATOM	437	CE	LYS	26	-0.716 -
11.505	-8.910	1 00	0.00	BrD ATOM	438	HE1	LYS	26	0 003 -
10 782	-9.266	1.00	0.00	BrD ATOM	439	HE2	LYS	26	-1.703 -
11.228	-9 249	1.00	0.00	BrD ATOM	440	NZ	LYS	26	-0.371 -
12.844	-9.465	1.00	0.00	BrD ATOM	441	HZ1	LYS	26	-1.215 -
13.285	-9.884	1.00	0.00	BrD ATOM	442	HZ2	LYS	26	-0.010 -
13 461	-8 710	1 00	0 00	BrD ATOM	443	HZ3	LYS	26	0 358 -
12 749	-10 199	1 00	0 00	BrD ATOM	444	C	LYS	26	-4 673 -
11.073	-5 468	1 00	0 00	BrD ATOM	445	O	LYS	26	-5 762 -
10.991	-6.036	1 00	0 00	BrD ATOM	446	N	SER	27	-4 315 -
12.118	-4.732	1 00	0.00	BrD ATOM	447	HN	SER	27	-3 439 -
12.109	-4 293	1 00	0 00	BrD ATOM	448	CA	SER	27	-5.204 -
13.257	-4 516	1 00	0 00	BrD ATOM	449	HA	SER	27	-6 104 -
13.100	-5 091	1.00	0 00	BrD ATOM	450	CB	SER	27	-4 532 -
14.553	-4 976	1 00	0 00	BrD ATOM	451	HB1	SER	27	-3 629 -
14 710	-4 404	1 00	0 00	BrD ATOM	452	HB2	SER	27	-5 207 -
15 381	-4 818	1 00	0 00	BrD ATOM	453	OG	SER	27	-4 197 -
14 492	-6 351	1 00	0.00	BrD ATOM	454	HG	SER	27	-3 746 -
15 300	-6.606	1 00	0 00	BrD ATOM	455	C	SER	27	-5 591 -
13 361	-3 050	1 00	0.00	BrD ATOM	456	O	SER	27	-5 962 -
14.431	-2 567	1 00	0.00	BrD ATOM	457	N	HIS	28	-5 477 -
12 246	-2 339	1 00	0 00	BrD ATOM	458	HN	HIS	28	-5 215 -
11.418	-2 785	1 00	0 00	BrD ATOM	459	CA	HIS	28	-5 863 -
12 197	-0.946	1 00	0 00	BrD ATOM	460	HA	HIS	28	-5 597 -
13.142	-0 497	1 00	0 00	BrD ATOM	461	CB	HIS	28	-5 125 -
11 076	-0 217	1 00	0 00	BrD ATOM	462	HB1	HIS	28	-4 073 -
11 308	-0 210	1 00	0 00	BrD ATOM	463	HB2	HIS	28	-5 283 -
10 146	-0.742	1 00	0 00	BrD ATOM	464	CG	HIS	28	-5 549 -
10.884	1 205	1 00	0 00	BrD ATOM	465	ND1	HIS	28	-5 742 -
11 931	2 081	1 00	0 00	BrD ATOM	466	HD1	HIS	28	-5 645 -
12 883	1 866	1 00	0 00	BrD ATOM	467	CD2	HIS	28	-5 780 -
9 754	1 916	1 00	0 00	BrD ATOM	468	HD2	HIS	28	-5 717 -
8 739	1 549	1 00	0 00	BrD ATOM	469	CE1	HIS	28	-6 092 -
11 456	3 262	1 00	0.00	BrD ATOM	470	HE1	HIS	28	-6 314 -
12 044	4 141	1.00	0 00	BrD ATOM	471	NE2	HIS	28	-6 119 -
10.139	3.189	1 00	0 00	BrD ATOM	472	HE2	HIS	28	-6 350 -
9 536	3.925	1 00	0 00	BrD ATOM	473	C	HIS	28	-7 364 -
12 017	-0 850	1 00	0 00	BrD ATOM	474	O	HIS	28	-7 979 -
11 356	-1 686	1 00	0 00	BrD ATOM	475	N	GLN	29	-7 954 -
12 666	0 128	1 00	0 00	BrD ATOM	476	HN	GLN	29	-7 404 -
13 189	0 747	1 00	0 00	BrD ATOM	477	CA	GLN	29	-9 397 -
12 630	0 298	1 00	0 00	BrD ATOM	478	HA	GLN	29	-9 836 -
12 688	-0 687	1 00	0 00	BrD ATOM	479	CB	GLN	29	-9 840 -
13 850	1 090	1 00	0 00	BrD ATOM	480	HB1	GLN	29	-9 485 -
13.761	2 106	1 00	0 00	BrD ATOM	481	HB2	GLN	29	-10 918 -
13.901	1 092	1 00	0 00	BrD ATOM	482	CG	GLN	29	-9 294 -
15 138	0 496	1 00	0 00	BrD ATOM	483	HG1	GLN	29	-8 707 -
14 887	-0 386	1 00	0 00	BrD ATOM	484	HG2	GLN	29	-8 660 -
15 618	1 227	1 00	0 00	BrD ATOM	485	CD	GLN	29	-10 390 -
16.105	0 093	1 00	0 00	BrD ATOM	486	OE1	GLN	29	-10 358 -
16 679	-0 996	1 00	0 00	BrD ATOM	487	NE2	GLN	29	-11 368 -
16 290	0 971	1 00	0 00	BrD ATOM	488	HE21	GLN	29	-12 090 -
16 910	0 737	1 00	0 00	BrD ATOM	489	HE22	GLN	29	-11 329 -
15 800	1 819	1 00	0 00	BrD ATOM	490	C	GLN	29	-9 866 -
11 332	0 951	1 00	0 00	BrD ATOM	491	O	GLN	29	-11 065 -
11 111	1 116	1 00	0 00	BrD ATOM	492	N	SER	30	-8 921 -
10 450	1 262	1 00	0 00	BrD ATOM	493	HN	SER	30	-7 985 -
10 661	1 074	1.00	0 00	BrD ATOM	494	CA	SER	30	-9 246 -
9.143	1 805	1.00	0 00	BrD ATOM	495	HA	SER	30	-10.319 -
9.036	1 787	1 00	0.00	BrD ATOM	496	CB	SER	30	-8.759 -
9 026	3 250	1 00	0 00	BrD ATOM	497	HB1	SER	30	-7 829 -
8 479	3 271	1 00	0.00	BrD ATOM	498	HB2	SER	30	-9 499 -
8 500	3 835	1 00	0.00	BrD ATOM	499	OG	SER	30	-8.552 -
10.307	3 823	1 00	0 00	BrD ATOM	500	HG	SER	30	-9 322 -
10.857	3 664	1 00	0.00	BrD ATOM	501	C	SER	30	-8 627 -
8.036	0.945	1 00	0.00	BrD ATOM	502	O	SER	30	-8 726 -
6 855	1 276	1 00	0.00	BrD ATOM	503	N	ALA	31	-7 977 -
8 425	-0 157	1 00	0 00	BrD ATOM	504	HN	ALA	31	-7 935 -
9 377	-0 385	1 00	0.00	BrD ATOM	505	CA	ALA	31	-7 365 -
7.462	-1.066	1 00	0 00	BrD ATOM	506	HA	ALA	31	-6 927 -
6.675	-0 470	1 00	0 00	BrD ATOM	507	CB	ALA	31	-6 251 -
8.123	-1 861	1.00	0 00	BrD ATOM	508	HB1	ALA	31	-5 395 -
8 274	-1 223	1 00	0 00	BrD ATOM	509	HB2	ALA	31	-5 974 -
7.489	-2 691	1 00	0 00	BrD ATOM	510	HB3	ALA	31	-6 593 -
9 076	-2 236	1 00	0 00	BrD ATOM	511	C	ALA	31	-8 397 -
6 851	-2.014	1.00	0.00	BrD ATOM	512	O	ALA	31	-8 097 -
5 900	-2 736	1 00	0 00	BrD ATOM	513	N	TRP	32	-9 614 -
7.396	-2 010	1.00	0 00	BrD ATOM	514	HN	TRP	32	-9 795 -
8 160	-1.427	1.00	0 00	BrD ATOM	515	CA	TRP	32	-10 669 -
6 906	-2 893	1 00	0 00	BrD ATOM	516	HA	TRP	32	-10.362 -
7 135	-3 902	1.00	0 00	BrD ATOM	517	CB	TRP	32	-12 002 -
7 630	-2 628	1.00	0.00	BrD ATOM	518	HB1	TRP	32	-12 770 -
7 192	-3 249	1 00	0.00	BrD ATOM	519	HB2	TRP	32	-11 894 -
8 671	-2 881	1 00	0 00	BrD ATOM	520	CG	TRP	32	-12 454 -
7 544	-1 209	1 00	0 00	BrD ATOM	521	CD1	TRP	32	-12 415 -
8 532	-0.267	1 00	0 00	BrD ATOM	522	HD1	TRP	32	-12 058 -
9.535	-0 450	1 00	0.00	BrD ATOM	523	CD2	TRP	32	-12 993 -
6.393	-0 565	1 00	0 00	BrD ATOM	524	NE1	TRP	32	-12 895 -
8 057	0 929	1.00	0 00	BrD ATOM	525	HE1	TRP	32	-12 970 -
8.574	1.758	1 00	0 00	BrD ATOM	526	CE2	TRP	32	-13.253 -
6.743	0 770	1 00	0 00	BrD ATOM	527	CE3	TRP	32	-13 270 -
5.095	-0 991	1 00	0.00	BrD ATOM	528	HE3	TRP	32	-13 068 -
4.788	-2 006	1.00	0 00	BrD ATOM	529	CZ2	TRP	32	-13 784 -
5.839	1.681	1.00	0.00	BrD ATOM	530	HZ2	TRP	32	-13 983 -
6.109	2 708	1 00	0.00	BrD ATOM	531	CZ3	TRP	32	-13 786 -
4.196	-0 086	1 00	0.00	BrD ATOM	532	HZ3	TRP	32	-14 003 -
3.185	-0 396	1.00	0.00	BrD ATOM	533	CH2	TRP	32	-14.055 -
4.577	1 230	1.00	0 00	BrD ATOM	534	HH2	TRP	32	-14 420 -

3.838	1.903	1.00	0.00	BrD ATOM	535	C	TRP	32	-10.855
5.382	-2.797	1.00	0.00	BrD ATOM	536	O	TRP	32	-11.199
4 752	-3 797	1 00	0.00	BrD ATOM	537	N	PRO	33	-10 636
4 741	-1 618	1.00	0 00	BrD ATOM	538	CA	PRO	33	-10 800
3 297	-1 493	1 00	0 00	BrD ATOM	539	HA	PRO	33	-11.693
2 959	-1 999	1 00	0.00	BrD ATOM	540	CB	PRO	33	-10 947
3 057	0 017	1 00	0 00	BrD ATOM	541	HB1	PRO	33	-10 191
2 357	0 341	1 00	0 00	BrD ATOM	542	HB2	PRO	33	-11 926
2 646	0 219	1 00	0.00	BrD ATOM	543	CG	PRO	33	-10 771
4.386	0 685	1 00	0 00	BrD ATOM	544	HG1	PRO	33	-11 713
4.744	1.048	1 00	0 00	BrD ATOM	545	HG2	PRO	33	-10.075
4 288	1 505	1.00	0 00	BrD ATOM	546	CD	PRO	33	-10 223
5 333	-0 337	1 00	0.00	BrD ATOM	547	HD1	PRO	33	-10 632
6 319	-0 205	1.00	0.00	BrD ATOM	548	HD2	PRO	33	-9 165
5 358	-0.254	1 00	0.00	BrD ATOM	549	C	PRO	33	-9 596
2 535	-2 040	1 00	0.00	BrD ATOM	550	O	PRO	33	-9.687
1 343	-2 332	1 00	0.00	BrD ATOM	551	N	PHE	34	-8 472
3 233	-2 187	1 00	0.00	BrD ATOM	552	HN	PHE	34	-8 458
4 180	-1 936	1 00	0.00	BrD ATOM	553	CA	PHE	34	-7.256
2 619	-2.703	1 00	0 00	BrD ATOM	554	HA	PHE	34	-7 295
1 564	-2 475	1 00	0 00	BrD ATOM	555	CB	PHE	34	-6 026
3 228	-2.030	1 00	0 00	BrD ATOM	556	HB1	PHE	34	-5 773
4 150	-2 531	1 00	0 00	BrD ATOM	557	HB2	PHE	34	-5 198
2 540	-2 118	1 00	0 00	BrD ATOM	558	CG	PHE	34	-6 228
3 531	-0 573	1.00	0 00	BrD ATOM	559	CD1	PHE	34	-6 985
2 689	0 226	1 00	0 00	BrD ATOM	560	HD1	PHE	34	-7 430
1.805	-0 208	1.00	0 00	BrD ATOM	561	CD2	PHE	34	-5 663
4 659	-0 003	1.00	0.00	BrD ATOM	562	HD2	PHE	34	-5 074
5 324	-0 617	1 00	0 00	BrD ATOM	563	CE1	PHE	34	-7 175
2 968	1 566	1 00	0 00	BrD ATOM	564	HE1	PHE	34	-7 767
2.303	2 179	1 00	0 00	BrD ATOM	565	CE2	PHE	34	-5 852
4 944	1 335	1 00	0.00	BrD ATOM	566	HE2	PHE	34	-5 409
5 829	1 765	1 00	0 00	BrD ATOM	567	CZ	PHE	34	-6 607
4 098	2 122	1 00	0.00	BrD ATOM	568	HZ	PHE	34	-6 753
4 319	3 168	1 00	0 00	BrD ATOM	569	C	PHE	34	-7 150
2 790	-4 213	1 00	0 00	BrD ATOM	570	O	PHE	34	-6 653
1 909	-4.907	1 00	0 00	BrD ATOM	571	N	MET	35	-7 624
3 923	-4 721	1 00	0 00	BrD ATOM	572	HN	MET	35	-8 000
4 598	-4 119	1 00	0.00	BrD ATOM	573	CA	MET	35	-7 545
4 205	-6 151	1 00	0 00	BrD ATOM	574	HA	MET	35	-6 600
3 825	-6 507	1 00	0 00	BrD ATOM	575	CB	MET	35	-7 593
5 706	-6 393	1 00	0 00	BrD ATOM	576	HB1	MET	35	-7 670
5 889	-7 454	1 00	0 00	BrD ATOM	577	HB2	MET	35	-8 463
6 114	-5 899	1.00	0 00	BrD ATOM	578	CG	MET	35	-6 367
6 423	-5 871	1.00	0 00	BrD ATOM	579	HG1	MET	35	-6 673
7 114	-5.107	1.00	0 00	BrD ATOM	580	HG2	MET	35	-5 696
5 692	-5 444	1 00	0.00	BrD ATOM	581	SD	MET	35	-5 490
7 322	-7 161	1 00	0 00	BrD ATOM	582	CE	MET	35	-4 032
6 298	-7 337	1 00	0 00	BrD ATOM	583	HE1	MET	35	-3 284
6 831	-7 905	1 00	0 00	BrD ATOM	584	HE2	MET	35	-3.639
6 062	-6 358	1 00	0.00	BrD ATOM	585	HE3	MET	35	-4 294
5 384	-7 850	1 00	0 00	BrD ATOM	586	C	MET	35	-8 661
3 519	-6 924	1 00	0 00	BrD ATOM	587	O	MET	35	-9 396
4 160	-7 675	1.00	0 00	BrD ATOM	588	N	GLU	36	-8 749
2 208	-6 762	1.00	0.00	BrD ATOM	589	HN	GLU	36	-8 116
1 765	-6 164	1.00	0.00	BrD ATOM	590	CA	GLU	36	-9 751
1 407	-7 457	1 00	0 00	BrD ATOM	591	HA	GLU	36	-9 531
1 453	-8 515	1 00	0 00	BrD ATOM	592	CB	GLU	36	-11 156
1.964	-7.207	1 00	0.00	BrD ATOM	593	HB1	GLU	36	-11 084
3 018	-6 987	1 00	0 00	BrD ATOM	594	HB2	GLU	36	-11 581
1 458	-6 354	1 00	0 00	BrD ATOM	595	CG	GLU	36	-12.099
1 787	-8 385	1 00	0 00	BrD ATOM	596	HG1	GLU	36	-11 527
1 466	-9 243	1 00	0 00	BrD ATOM	597	HG2	GLU	36	-12 569
2 735	-8 600	1 00	0 00	BrD ATOM	598	CD	GLU	36	-13 182
0 761	-8.114	1 00	0 00	BrD ATOM	599	OE1	GLU	36	-12.865
0 447	-8 098	1 00	0 00	BrD ATOM	600	OE2	GLU	36	-14.348
1 165	-7 919	1 00	0 00	BrD ATOM	601	C	GLU	36	-9.692
0 050	-7 001	1 00	0 00	BrD ATOM	602	O	GLU	36	-10 470
0 471	-6 145	1 00	0 00	BrD ATOM	603	N	PRO	37	-8 764
0 842	-7 565	1 00	0 00	BrD ATOM	604	CA	PRO	37	-8 604
2 255	-7 202	1 00	0 00	BrD ATOM	605	HA	PRO	37	-8 407
2 369	-6 146	1 00	0 00	BrD ATOM	606	CB	PRO	37	-7 376
2 709	-8 004	1 00	0 00	BrD ATOM	607	HB1	PRO	37	-7 696
3 306	-8 846	1 00	0 00	BrD ATOM	608	HB2	PRO	37	-6 728
3 295	-7 370	1 00	0 00	BrD ATOM	609	CG	PRO	37	-6 706
1 453	-8 451	1 00	0 00	BrD ATOM	610	HG1	PRO	37	-6 222
1 614	-9.403	1 00	0 00	BrD ATOM	611	HG2	PRO	37	-5 984
1 139	-7 711	1 00	0.00	BrD ATOM	612	CD	PRO	37	-7.793
0 426	-8 587	1 00	0 00	BrD ATOM	613	HD1	PRO	37	-8 229
0 465	-9 574	1 00	0 00	BrD ATOM	614	HD2	PRO	37	-7 410
0 561	-8 378	1 00	0.00	BrD ATOM	615	C	PRO	37	-9.822
3 093	-7 576	1 00	0 00	BrD ATOM	616	O	PRO	37	-10.678
2 655	-8 344	1 00	0 00	BrD ATOM	617	N	VAL	38	-9 892
4 301	-7 025	1 00	0 00	BrD ATOM	618	HN	VAL	38	-9 179
4 594	-6 422	1 00	0 00	BrD ATOM	619	CA	VAL	38	-11.006
5 206	-7 300	1.00	0 00	BrD ATOM	620	HA	VAL	38	-11 709
4 683	-7 931	1 00	0 00	BrD ATOM	621	CB	VAL	38	-11 750
5 646	-6 012	1 00	0 00	BrD ATOM	622	HB	VAL	38	-11 449
6 657	-5 781	1 00	0 00	BrD ATOM	623	CG1	VAL	38	-11 395
4 767	-4.819	1 00	0.00	BrD ATOM	624	HG11	VAL	38	-11.888
5.145	-3 935	1 00	0 00	BrD ATOM	625	HG12	VAL	38	-10 326
4 779	-4.667	1 00	0.00	BrD ATOM	626	HG13	VAL	38	-11 721
3 755	-5 008	1.00	0.00	BrD ATOM	627	CG2	VAL	38	-13 253
5 646	-6 246	1.00	0 00	BrD ATOM	628	HG21	VAL	38	-13 760
5.374	-5.333	1.00	0.00	BrD ATOM	629	HG22	VAL	38	-13.497
4.934	-7.020	1.00	0.00	BrD ATOM	630	HG23	VAL	38	-13.570
6 629	-6 553	1 00	0 00	BrD ATOM	631	C	VAL	38	-10 518
6.451	-8 035	1.00	0.00	BrD ATOM	632	O	VAL	38	-9 410
6 473	-8 571	1.00	0 00	BrD ATOM	633	N	LYS	39	-11 349
7.488	-8.051	1 00	0 00	BrD ATOM	634	HN	LYS	39	-12 215
7.412	-7 609	1 00	0 00	BrD ATOM	635	CA	LYS	39	-11 005
8 737	-8 715	1 00	0 00	BrD ATOM	636	HA	LYS	39	-9 947
8 906	-8 574	1 00	0 00	BrD ATOM	637	CB	LYS	39	-11 299
8 646	-10 216	1 00	0.00	BrD ATOM	638	HB1	LYS	39	-10.419
8 285	-10 714	1 00	0 00	BrD ATOM	639	HB2	LYS	39	-11 531
9 633	-10 587	1 00	0.00	BrD ATOM	640	CG	LYS	39	-12 452
7 722	-10 569	1 00	0 00	BrD ATOM	641	HG1	LYS	39	-12 970
7 450	-9 664	1 00	0 00	BrD ATOM	642	HG2	LYS	39	-13.127
8 241	-11 232	1 00	0 00	BrD ATOM	643	CD	LYS	39	-11.962
6 458	-11 256	1.00	0 00	BrD ATOM	644	HD1	LYS	39	-12 413
5 601	-10 777	1 00	0 00	BrD ATOM	645	HD2	LYS	39	-10 888
6 402	-11 160	1.00	0.00	BrD ATOM	646	CE	LYS	39	-12 326
6 447	-12 732	1 00	0.00	BrD ATOM	647	HE1	LYS	39	-11 779
5 653	-13 219	1 00	0 00	BrD ATOM	648	HE2	LYS	39	-12 044
7 395	-13 166	1 00	0.00	BrD ATOM	649	NZ	LYS	39	-13 784
6 232	-12.945	1 00	0 00	BrD ATOM	650	HZ1	LYS	39	-13 963
5 950	-13 930	1 00	0 00	BrD ATOM	651	HZ2	LYS	39	-14 307
7.108	-12 745	1 00	0.00	BrD ATOM	652	HZ3	LYS	39	-14 130
5 482	-12.313	1 00	0 00	BrD ATOM	653	C	LYS	39	-11 772
9 903	-8 105	1 00	0 00	BrD ATOM	654	O	LYS	39	-12 487
9 739	-7 116	1 00	0 00	BrD ATOM	655	N	ARG	40	-11 626
11 078	-8 706	1 00	0 00	BrD ATOM	656	HN	ARG	40	-11 040
11 146	-9 488	1 00	0 00	BrD ATOM	657	CA	ARG	40	-12 304
12 273	-8 223	1 00	0 00	BrD ATOM	658	HA	ARG	40	-12 018
12 419	-7 191	1.00	0 00	BrD ATOM	659	CB	ARG	40	-11.866
13.492	-9 037	1 00	0 00	BrD ATOM	660	HB1	ARG	40	-12 313
13 435	-10 019	1 00	0.00	BrD ATOM	661	HB2	ARG	40	-10 792
13 476	-9 139	1 00	0.00	BrD ATOM	662	CG	ARG	40	-12 265
14 819	-8 410	1.00	0 00	BrD ATOM	663	HG1	ARG	40	-12 664
14 634	-7 424	1 00	0 00	BrD ATOM	664	HG2	ARG	40	-13.020
15 285	-9 025	1 00	0 00	BrD ATOM	665	CD	ARG	40	-11 075
15 759	-8 292	1 00	0 00	BrD ATOM	666	HD1	ARG	40	-10.715
15.988	-9 284	1 00	0 00	BrD ATOM	667	HD2	ARG	40	-10 296
15 263	-7 732	1 00	0 00	BrD ATOM	668	NE	ARG	40	-11 426
17 004	-7 616	1 00	0 00	BrD ATOM	669	HE	ARG	40	-11 554
17 802	-8 171	1 00	0 00	BrD ATOM	670	CZ	ARG	40	-11 577
17 109	-6 300	1 00	0 00	BrD ATOM	671	NH1	ARG	40	-11 409
16 047	-5 525	1 00	0 00	BrD ATOM	672	HH11	ARG	40	-11 168
15 165	-5 930	1 00	0 00	BrD ATOM	673	HH12	ARG	40	-11 523
16.127	-4 535	1 00	0.00	BrD ATOM	674	NH2	ARG	40	-11 897
18 276	-5 758	1 00	0.00	BrD ATOM	675	HH21	ARG	40	-12.011
18 353	-4 767	1 00	0 00	BrD ATOM	676	HH22	ARG	40	-12 025
19 079	-6.339	1 00	0 00	BrD ATOM	677	C	ARG	40	-13 824
12 123	-8 293	1 00	0.00	BrD ATOM	678	O	ARG	40	-14.556
12 915	-7 700	1 00	0 00	BrD ATOM	679	N	THR	41	-14.301
11 109	-9 017	1 00	0 00	BrD ATOM	680	HN	THR	41	-13 680
10 511	-9 481	1 00	0 00	BrD ATOM	681	CA	THR	41	-15 737
10 898	-9 159	1 00	0 00	BrD ATOM	682	HA	THR	41	-16 228
11 725	-8 681	1 00	0 00	BrD ATOM	683	CB	THR	41	-16 133
10 870	-10 637	1 00	0 00	BrD ATOM	684	HB	THR	41	-15.862
11 812	-11 090	1 00	0.00	BrD ATOM	685	OG1	THR	41	-17.533
10 696	-10 775	1 00	0 00	BrD ATOM	686	HG1	THR	41	-17.988
11 239	-10 127	1 00	0 00	BrD ATOM	687	CG2	THR	41	-15.453
9 771	-11 421	1 00	0 00	BrD ATOM	688	HG21	THR	41	-14 433
9 669	-11 083	1.00	0.00	BrD ATOM	689	HG22	THR	41	-15 462
10 020	-12 472	1.00	0.00	BrD ATOM	690	HG23	THR	41	-15 979
8 841	-11 267	1 00	0.00	BrD ATOM	691	C	THR	41	-16 197
9 623	-8 467	1 00	0 00	BrD ATOM	692	O	THR	41	-17 123
9 656	-7 658	1 00	0 00	BrD ATOM	693	N	GLU	42	-15 573
8 498	-8 792	1 00	0 00	BrD ATOM	694	HN	GLU	42	-14 835
8 521	-9.435	1 00	0 00	BrD ATOM	695	CA	GLU	42	-15 940
7 236	-8 163	1 00	0 00	BrD ATOM	696	HA	GLU	42	-16.954
7 002	-8.454	1 00	0 00	BrD ATOM	697	CB	GLU	42	-15.013
6 109	-8 623	1 00	0.00	BrD ATOM	698	HB1	GLU	42	-15 239
5 220	-8 053	1 00	0 00	BrD ATOM	699	HB2	GLU	42	-13 993
6 398	-8 431	1 00	0 00	BrD ATOM	700	CG	GLU	42	-15 142
5 774	-10 098	1 00	0 00	BrD ATOM	701	HG1	GLU	42	-14 284
5 191	-10 396	1 00	0 00	BrD ATOM	702	HG2	GLU	42	-15 166
6 694	-10 663	1 00	0.00	BrD ATOM	703	CD	GLU	42	-16 397
4 982	-10 409	1 00	0 00	BrD ATOM	704	OE1	GLU	42	-17 489
5 589	-10 443	1.00	0.00	BrD ATOM	705	OE2	GLU	42	-16 289
3 756	-10 620	1 00	0.00	BrD ATOM	706	C	GLU	42	-15 881
7 374	-6 647	1 00	0 00	BrD ATOM	707	O	GLU	42	-16 614
6 703	-5 920	1 00	0 00	BrD ATOM	708	N	ALA	43	-15 024
8 279	-6 181	1 00	0 00	BrD ATOM	709	HN	ALA	43	-14 457
8 774	-6 817	1 00	0 00	BrD ATOM	710	CA	ALA	43	-14 861
8 509	-4 752	1 00	0 00	BrD ATOM	711	HA	ALA	43	-15.712
8 080	-4 245	1 00	0 00	BrD ATOM	712	CB	ALA	43	-13 609
7.810	-4 245	1 00	0.00	BrD ATOM	713	HB1	ALA	43	-12 893
7 731	-5 049	1 00	0 00	BrD ATOM	714	HB2	ALA	43	-13 866
6 822	-3 893	1 00	0 00	BrD ATOM	715	HB3	ALA	43	-13 180
8 381	-3 435	1 00	0 00	BrD ATOM	716	C	ALA	43	-14.799
10 002	-4.440	1 00	0 00	BrD ATOM	717	O	ALA	43	-13 721
10 555	-4 222	1.00	0.00	BrD ATOM	718	N	PRO	44	-15.962
10 676	-4 414	1 00	0.00	BrD ATOM	719	CA	PRO	44	-16 038
12 114	-4 129	1.00	0 00	BrD ATOM	720	HA	PRO	44	-15 511
12 692	-4 874	1.00	0 00	BrD ATOM	721	CB	PRO	44	-17 539
12 422	-4 207	1 00	0 00	BrD ATOM	722	HB1	PRO	44	-17 688
13.369	-4.704	1.00	0.00	BrD ATOM	723	HB2	PRO	44	-17.951
12.465	-3.210	1.00	0.00	BrD ATOM	724	CG	PRO	44	-18.125
11 298	-4 991	1 00	0 00	BrD ATOM	725	HG1	PRO	44	-18 071
11 518	-6 047	1 00	0.00	BrD ATOM	726	HG2	PRO	44	-19 150
11 137	-4 692	1 00	0 00	BrD ATOM	727	CD	PRO	44	-17 291
10 095	-4 665	1 00	0 00	BrD ATOM	728	HD1	PRO	44	-17 264
9 413	-5 500	1 00	0 00	BrD ATOM	729	HD2	PRO	44	-17 668
9 601	-3 783	1 00	0 00	BrD ATOM	730	C	PRO	44	-15 498
12 458	-2 746	1 00	0 00	BrD ATOM	731	O	PRO	44	-16 262
12 635	-1 797	1.00	0 00	BrD ATOM	732	N	GLY	45	-14 177
12 551	-2 637	1 00	0 00	BrD ATOM	733	HN	GLY	45	-13 617
12 400	-3 427	1 00	0 00	BrD ATOM	734	CA	GLY	45	-13 560
12 875	-1 365	1 00	0 00	BrD ATOM	735	HA1	GLY	45	-13 586
13 946	-1.228	1.00	0 00	BrD ATOM	736	HA2	GLY	45	-14.128
12 409	-0 573	1 00	0 00	BrD ATOM	737	C	GLY	45	-12.121
12 405	-1 278	1 00	0.00	BrD ATOM	738	O	GLY	45	-11 333
12 942	-0 499	1 00	0 00	BrD ATOM	739	N	TYR	46	-11 777
11 403	-2 081	1.00	0 00	BrD ATOM	740	HN	TYR	46	-12 450
11 015	-2 678	1 00	0 00	BrD ATOM	741	CA	TYR	46	-10 423
10.861	-2 089	1 00	0 00	BrD ATOM	742	HA	TYR	46	-10 271
10 337	-1 158	1 00	0 00	BrD ATOM	743	CB	TYR	46	-10 255
9 878	-3 249	1 00	0 00	BrD ATOM	744	HB1	TYR	46	-11 073
10 006	-3 942	1 00	0 00	BrD ATOM	745	HB2	TYR	46	-9 324
10.084	-3 755	1 00	0 00	BrD ATOM	746	CG	TYR	46	-10 237
8 431	-2 814	1 00	0 00	BrD ATOM	747	CD1	TYR	46	-9.262
7 558	-3.279	1 00	0 00	BrD ATOM	748	HD1	TYR	46	-8 511
7 926	-3 962	1 00	0 00	BrD ATOM	749	CD2	TYR	46	-11 194
7 938	-1 935	1 00	0 00	BrD ATOM	750	HD2	TYR	46	-11 958
8 605	-1 564	1 00	0 00	BrD ATOM	751	CE1	TYR	46	-9 242
6 235	-2 884	1 00	0 00	BrD ATOM	752	HE1	TYR	46	-8 474
5 572	-3 254	1 00	0 00	BrD ATOM	753	CE2	TYR	46	-11 180
6 617	-1 534	1 00	0 00	BrD ATOM	754	HE2	TYR	46	-11 933
6 253	-0 850	1 00	0 00	BrD ATOM	755	CZ	TYR	46	-10 203
5 769	-2 010	1 00	0 00	BrD ATOM	756	OH	TYR	46	-10 186
4 452	-1 612	1 00	0 00	BrD ATOM	757	HH	TYR	46	-9 895
4 397	-0 699	1 00	0 00	BrD ATOM	758	C	TYR	46	-9.386
11 975	-2 200	1.00	0.00	BrD ATOM	759	O	TYR	46	-9 727
13 132	-2 446	1 00	0 00	BrD ATOM	760	N	TYR	47	-8 120
11 618	-2 014	1 00	0.00	BrD ATOM	761	HN	TYR	47	-7 911
10 680	-1 823	1 00	0.00	BrD ATOM	762	CA	TYR	47	-7 033
12 587	-2 097	1 00	0 00	BrD ATOM	763	HA	TYR	47	-6 102
12 042	-2 050	1 00	0.00	BrD ATOM	764	CB	TYR	47	-7 099
13 345	-3 424	1 00	0 00	BrD ATOM	765	HB1	TYR	47	-7 889
14 080	-3 370	1 00	0 00	BrD ATOM	766	HB2	TYR	47	-6 158
13 848	-3 590	1 00	0 00	BrD ATOM	767	CG	TYR	47	-7 370
12 459	-4 619	1 00	0.00	BrD ATOM	768	CD1	TYR	47	-8 056
12.946	-5 725	1 00	0 00	BrD ATOM	769	HD1	TYR	47	-8 397
13 971	-5 722	1 00	0 00	BrD ATOM	770	CD2	TYR	47	-6 940
11 137	-4.644	1 00	0 00	BrD ATOM	771	HD2	TYR	47	-6.405
10 742	-3 792	1 00	0 00	BrD ATOM	772	CE1	TYR	47	-8 306
12 143	-6 821	1 00	0.00	BrD ATOM	773	HE1	TYR	47	-8 841
12 540	-7 671	1 00	0 00	BrD ATOM	774	CE2	TYR	47	-7 186
10 328	-5 738	1.00	0 00	BrD ATOM	775	HE2	TYR	47	-6 845
9 303	-5 739	1 00	0 00	BrD ATOM	776	CZ	TYR	47	-7 870
10 835	-6 823	1 00	0 00	BrD ATOM	777	OH	TYR	47	-8 117
10 032	-7.912	1 00	0 00	BrD ATOM	778	HH	TYR	47	-7.572
10.317	-8 650	1 00	0.00	BrD ATOM	779	C	TYR	47	-7 085
13 572	-0 933	1.00	0 00	BrD ATOM	780	O	TYR	47	-6 183
13.605	-0 095	1.00	0 00	BrD ATOM	781	N	GLU	48	-8 144
14 376	-0.887	1 00	0 00	BrD ATOM	782	HN	GLU	48	-8 830
14 304	-1 584	1 00	0 00	BrD ATOM	783	CA	GLU	48	-8 309
15 365	0 174	1 00	0 00	BrD ATOM	784	HA	GLU	48	-7 569
16 138	0 024	1 00	0 00	BrD ATOM	785	CB	GLU	48	-9 704
15 991	0 104	1 00	0 00	BrD ATOM	786	HB1	GLU	48	-9 746
16 827	0 786	1 00	0 00	BrD ATOM	787	HB2	GLU	48	-10 432
15 254	0 408	1 00	0 00	BrD ATOM	788	CG	GLU	48	-10.079
16 488	-1 283	1 00	0 00	BrD ATOM	789	HG1	GLU	48	-9 268
17.086	-1 669	1 00	0 00	BrD ATOM	790	HG2	GLU	48	-10 235
15 635	-1 927	1 00	0 00	BrD ATOM	791	CD	GLU	48	-11 341
17 328	-1.282	1.00	0.00	BrD ATOM	792	OE1	GLU	48	-12 059
17.320	-0.260	1.00	0 00	BrD ATOM	793	OE2	GLU	48	-11 612
17.994	-2.304	1.00	0.00	BrD ATOM	794	C	GLU	48	-8 091
14.736	1.547	1 00	0 00	BrD ATOM	795	O	GLU	48	-7.683
15.410	2 493	1 00	0 00	BrD ATOM	796	N	VAL	49	-8 360
13 439	1 645	1 00	0 00	BrD ATOM	797	HN	VAL	49	-8 682
12.958	0 854	1 00	0 00	BrD ATOM	798	CA	VAL	49	-8 192
12.712	2 899	1 00	0 00	BrD ATOM	799	HA	VAL	49	-7 919
13 423	3 665	1.00	0.00	BrD ATOM	800	CB	VAL	49	-9 495
12 010	3 332	1 00	0 00	BrD ATOM	801	HB	VAL	49	-9 555
11 064	2 815	1 00	0.00	BrD ATOM	802	CG1	VAL	49	-10.713
12.834	2.949	1.00	0 00	BrD ATOM	803	HG11	VAL	49	-11 006
12.591	1 937	1.00	0.00	BrD ATOM	804	HG12	VAL	49	-10 472
13.884	3 011	1 00	0.00	BrD ATOM	805	HG13	VAL	49	-11 526
12 609	3 622	1 00	0.00	BrD ATOM	806	CG2	VAL	49	-9 475
11.729	4.827	1.00	0 00	BrD ATOM	807	HG21	VAL	49	-9.393
12 661	5 367	1 00	0 00	BrD ATOM	808	HG22	VAL	49	-8.628
11.101	5 062	1.00	0 00	BrD ATOM	809	HG23	VAL	49	-10 387
11.226	5 111	1 00	0 00	BrD ATOM	810	C	VAL	49	-7 100
11.656	2.787	1 00	0 00	BrD ATOM	811	O	VAL	49	-6 592
11 167	3 797	1 00	0 00	BrD ATOM	812	N	ILE	50	-6 763
11.281	1 558	1 00	0.00	BrD ATOM	813	HN	ILE	50	-7 214
11.686	0 792	1 00	0 00	BrD ATOM	814	CA	ILE	50	-5.769
10.245	1 324	1 00	0 00	BrD ATOM	815	HA	ILE	50	-5.542
9 783	2 274	1 00	0 00	BrD ATOM	816	CB	ILE	50	-6 291

9.152	0.366	1.00	0.00	BrD ATOM	817	HB	ILE	50	-6.001
9 428	-0 635	1 00	0.00	BrD ATOM	818	CG1	ILE	50	-7 818
9 035	0 436	1.00	0 00	BrD ATOM	819	HG11	ILE	50	-8 256
10 011	0.288	1.00	0.00	BrD ATOM	820	HG12	ILE	50	-8 158
8 371	-0 344	1 00	0 00	BrD ATOM	821	CG2	ILE	50	-5 644
7 815	0 684	1.00	0 00	BrD ATOM	822	HG21	ILE	50	-5.490
7 264	-0.233	1.00	0 00	BrD ATOM	823	HG22	ILE	50	-6 289
7 250	1 339	1 00	0 00	BrD ATOM	824	HG23	ILE	50	-4 694
7.981	1 169	1 00	0.00	BrD ATOM	825	CD1	ILE	50	-8.324
8 499	1 757	1 00	0.00	BrD ATOM	826	HD11	ILE	50	-8 330
9 293	2 489	1.00	0 00	BrD ATOM	827	HD12	ILE	50	-7.674
7 704	2 094	1.00	0 00	BrD ATOM	828	HD13	ILE	50	-9 326
8 116	1 631	1 00	0 00	BrD ATOM	829	C	ILE	50	-4 490
10.827	0 738	1 00	0 00	BrD ATOM	830	O	ILE	50	-4 504
11 444	-0 327	1 00	0.00	BrD ATOM	831	N	ARG	51	-3.384
10 597	1 428	1 00	0 00	BrD ATOM	832	HN	ARG	51	-3 443
10 086	2 260	1 00	0 00	BrD ATOM	833	CA	ARG	51	-2 082
11 061	0 969	1 00	0 00	BrD ATOM	834	HA	ARG	51	-2 068
12 139	1.024	1 00	0 00	BrD ATOM	835	CB	ARG	51	-0 988
10.491	1.870	1.00	0 00	BrD ATOM	836	HB1	ARG	51	-1 452
10 081	2 754	1 00	0 00	BrD ATOM	837	HB2	ARG	51	-0 478
9 698	1 341	1 00	0 00	BrD ATOM	838	CG	ARG	51	0 048
11 516	2 301	1 00	0.00	BrD ATOM	839	HG1	ARG	51	-0 399
12.185	3.022	1 00	0 00	BrD ATOM	840	HG2	ARG	51	0 883
11 000	2 753	1.00	0 00	BrD ATOM	841	CD	ARG	51	0 552
12 329	1 120	1 00	0 00	BrD ATOM	842	HD1	ARG	51	0.514
11 713	0.233	1 00	0 00	BrD ATOM	843	HD2	ARG	51	-0.090
13 187	0 989	1 00	0 00	BrD ATOM	844	NE	ARG	51	1.923
12 789	1 318	1.00	0 00	BrD ATOM	845	HE	ARG	51	2 296
12 730	2 222	1.00	0 00	BrD ATOM	846	CZ	ARG	51	2 683
13 279	0 344	1 00	0 00	BrD ATOM	847	NH1	ARG	51	3 921
13 678	0 602	1 00	0 00	BrD ATOM	848	HH11	ARG	51	4 491
14 046	-0 132	1 00	0 00	BrD ATOM	849	HH12	ARG	51	4 284
13 610	1 532	1 00	0 00	BrD ATOM	850	NH2	ARG	51	2 206
13 371	-0 890	1 00	0 00	BrD ATOM	851	HH21	ARG	51	2 779
13 739	-1 622	1 00	0 00	BrD ATOM	852	HH22	ARG	51	1 273
13 071	-1 089	1 00	0 00	BrD ATOM	853	C	ARG	51	-1.836
10 631	-0 471	1 00	0.00	BrD ATOM	854	O	ARG	51	-1 644
11.461	-1 360	1 00	0 00	BrD ATOM	855	N	SER	52	-1 843
9 322	-0.687	1 00	0 00	BrD ATOM	856	HN	SER	52	-2.010
8 718	0 067	1.00	0 00	BrD ATOM	857	CA	SER	52	-1 634
8.753	-2 012	1 00	0 00	BrD ATOM	858	HA	SER	52	-1 991
9 462	-2 740	1 00	0 00	BrD ATOM	859	CB	SER	52	-0 145
8 497	-2 253	1 00	0 00	BrD ATOM	860	HB1	SER	52	0 426
8 900	-1 430	1 00	0 00	BrD ATOM	861	HB2	SER	52	0.028
7 433	-2 325	1 00	0 00	BrD ATOM	862	OG	SER	52	0.290
9 112	-3 453	1 00	0 00	BrD ATOM	863	HG	SER	52	-0 218
8 768	-4 192	1 00	0 00	BrD ATOM	864	C	SER	52	-2 415
7 450	-2 148	1.00	0 00	BrD ATOM	865	O	SER	52	-1 912
6 382	-1 801	1 00	0.00	BrD ATOM	866	N	PRO	53	-3 675
7.518	-2 619	1 00	0.00	BrD ATOM	867	CA	PRO	53	-4 531
6 344	-2 745	1.00	0 00	BrD ATOM	868	HA	PRO	53	-4 993
6 101	-1 800	1 00	0 00	BrD ATOM	869	CB	PRO	53	-5.620
6 776	-3 738	1 00	0 00	BrD ATOM	870	HB1	PRO	53	-5 555
6 173	-4 630	1.00	0.00	BrD ATOM	871	HB2	PRO	53	-6 590
6 638	-3 284	1 00	0 00	BrD ATOM	872	CG	PRO	53	-5 371
8.224	-4 043	1 00	0 00	BrD ATOM	873	HG1	PRO	53	-6 296
8 775	-3 959	1 00	0 00	BrD ATOM	874	HG2	PRO	53	-4 969
8.321	-5 041	1 00	0 00	BrD ATOM	875	CD	PRO	53	-4 377
8 735	-3 034	1 00	0 00	BrD ATOM	876	HD1	PRO	53	-4 886
9 191	-2 200	1 00	0 00	BrD ATOM	877	HD2	PRO	53	-3 704
9 437	-3 498	1 00	0 00	BrD ATOM	878	C	PRO	53	-3 770
5 120	-3 252	1 00	0.00	BrD ATOM	879	O	PRO	53	-3.456
4 218	-2 475	1 00	0.00	BrD ATOM	880	N	MET	54	-3.471
5 089	-4 553	1 00	0 00	BrD ATOM	881	HN	MET	54	-3 738
5 838	-5 124	1 00	0 00	BrD ATOM	882	CA	MET	54	-2 734
3.970	-5 149	1 00	0 00	BrD ATOM	883	HA	MET	54	-2 905
3 995	-6 215	1 00	0 00	BrD ATOM	884	CB	MET	54	-1 236
4 127	-4 877	1.00	0 00	BrD ATOM	885	HB1	MET	54	-0 936
5 129	-5 145	1 00	0 00	BrD ATOM	886	HB2	MET	54	-1 057
3.978	-3 822	1 00	0.00	BrD ATOM	887	CG	MET	54	-0 368
3 147	-5 649	1 00	0 00	BrD ATOM	888	HG1	MET	54	-0 510
2 160	-5 235	1.00	0 00	BrD ATOM	889	HG2	MET	54	0 666
3 438	-5 537	1 00	0.00	BrD ATOM	890	SD	MET	54	-0 767
3 101	-7 407	1 00	0 00	BrD ATOM	891	CE	MET	54	-2 176
1.995	-7 401	1.00	0.00	BrD ATOM	892	HE1	MET	54	-2 086
1 294	-8 214	1.00	0 00	BrD ATOM	893	HE2	MET	54	-3 085
2 567	-7 518	1.00	0 00	BrD ATOM	894	HE3	MET	54	-2 208
1 457	-6 465	1 00	0 00	BrD ATOM	895	C	MET	54	-3 229
2 630	-4.602	1.00	0 00	BrD ATOM	896	O	MET	54	-2.556
1 990	-3 795	1.00	0 00	BrD ATOM	897	N	ASP	55	-4 422
2.232	-5.029	1 00	0 00	BrD ATOM	898	HN	ASP	55	-4 919
2.803	-5 652	1.00	0 00	BrD ATOM	899	CA	ASP	55	-5 045
1.005	-4 544	1.00	0 00	BrD ATOM	900	HA	ASP	55	-5.234
1.142	-3 490	1 00	0 00	BrD ATOM	901	CB	ASP	55	-6 391
0 793	-5 249	1 00	0 00	BrD ATOM	902	HB1	ASP	55	-6 327
0 045	-5 917	1 00	0.00	BrD ATOM	903	HB2	ASP	55	-6 631
1 679	-5 817	1.00	0.00	BrD ATOM	904	CG	ASP	55	-7 520
0 536	-4.269	1.00	0 00	BrD ATOM	905	OD1	ASP	55	-8 426
0 256	-4 602	1.00	0 00	BrD ATOM	906	OD2	ASP	55	-7.496
1 126	-3 169	1 00	0 00	BrD ATOM	907	C	ASP	55	-4.121
0 212	-4 704	1 00	0.00	BrD ATOM	908	O	ASP	55	-3 406
0 570	-3 772	1 00	0.00	BrD ATOM	909	N	LEU	56	-4.142
0 856	-5 870	1 00	0.00	BrD ATOM	910	HN	LEU	56	-4 715
0.533	-6.586	1.00	0.00	BrD ATOM	911	CA	LEU	56	-3.306
2.030	-6 111	1 00	0 00	BrD ATOM	912	HA	LEU	56	-2.301
1.790	-5 810	1 00	0 00	BrD ATOM	913	CB	LEU	56	-3 804
3 224	-5 292	1 00	0 00	BrD ATOM	914	HB1	LEU	56	-3.692
4 115	-5 892	1 00	0 00	BrD ATOM	915	HB2	LEU	56	-4.852
3 082	-5 089	1.00	0.00	BrD ATOM	916	CG	LEU	56	-3.088
3 451	-3 962	1.00	0 00	BrD ATOM	917	HG	LEU	56	-3 356
2.661	-3 279	1 00	0.00	BrD ATOM	918	CD1	LEU	56	-3 521
4.770	-3.344	1 00	0 00	BrD ATOM	919	HD11	LEU	56	-2 809
5 539	-3.606	1 00	0.00	BrD ATOM	920	HD12	LEU	56	-4 497
5.040	-3.719	1 00	0 00	BrD ATOM	921	HD13	LEU	56	-3 562
4 668	-2 270	1 00	0 00	BrD ATOM	922	CD2	LEU	56	-1 580
3 419	-4 153	1.00	0 00	BrD ATOM	923	HD21	LEU	56	-1 352
3 388	-5 209	1 00	0 00	BrD ATOM	924	HD22	LEU	56	-1 144
4 306	-3.716	1 00	0 00	BrD ATOM	925	HD23	LEU	56	-1 175
2 542	-3 671	1.00	0 00	BrD ATOM	926	C	LEU	56	-3 305
2 400	-7 587	1.00	0 00	BrD ATOM	927	O	LEU	56	-2 271
2 760	-8 150	1 00	0 00	BrD ATOM	928	N	LYS	57	-4 475
2 304	-8 207	1.00	0 00	BrD ATOM	929	HN	LYS	57	-5 261
2 020	-7.696	1 00	0 00	BrD ATOM	930	CA	LYS	57	-4 634
2 639	-9 615	1 00	0 00	BrD ATOM	931	HA	LYS	57	-4.577
3 712	-9 704	1 00	0 00	BrD ATOM	932	CB	LYS	57	-6 007
2 179	-10.108	1 00	0 00	BrD ATOM	933	HB1	LYS	57	-6.765
2 764	-9 608	1 00	0 00	BrD ATOM	934	HB2	LYS	57	-6 139
1 139	-9 850	1 00	0.00	BrD ATOM	935	CG	LYS	57	-6 203
2 328	-11 608	1 00	0 00	BrD ATOM	936	HG1	LYS	57	-5 383
1 845	-12 118	1 00	0 00	BrD ATOM	937	HG2	LYS	57	-7 132
1 856	-11 889	1.00	0 00	BrD ATOM	938	CD	LYS	57	-6 248
3 790	-12 024	1 00	0 00	BrD ATOM	939	HD1	LYS	57	-5 259
4 098	-12 327	1 00	0 00	BrD ATOM	940	HD2	LYS	57	-6 571
4 383	-11 181	1 00	0 00	BrD ATOM	941	CE	LYS	57	-7 210
4 011	-13 180	1 00	0 00	BrD ATOM	942	HE1	LYS	57	-7.354
3 073	-13.697	1 00	0 00	BrD ATOM	943	HE2	LYS	57	-6 778
4 732	-13.858	1 00	0 00	BrD ATOM	944	NZ	LYS	57	-8.532
4 515	-12 715	1 00	0 00	BrD ATOM	945	HZ1	LYS	57	-8.403
5 182	-11.928	1 00	0 00	BrD ATOM	946	HZ2	LYS	57	-9.022
5 003	-13 492	1 00	0 00	BrD ATOM	947	HZ3	LYS	57	-9 122
3 723	-12 391	1 00	0 00	BrD ATOM	948	C	LYS	57	-3 533
2 015	-10 473	1.00	0 00	BrD ATOM	949	O	LYS	57	-3 222
2 516	-11 553	1.00	0.00	BrD ATOM	950	N	THR	58	-2 941
0 923	-9 989	1 00	0.00	BrD ATOM	951	HN	THR	58	-3 240
0 552	-9 135	1 00	0 00	BrD ATOM	952	CA	THR	58	-1 901
0 230	-10 742	1 00	0 00	BrD ATOM	953	HA	THR	58	-1 819
0 717	-11 702	1 00	0.00	BrD ATOM	954	CB	THR	58	-2 307
1 233	-10 967	1 00	0 00	BrD ATOM	955	HB	THR	58	-2.611
1.660	-10 024	1 00	0 00	BrD ATOM	956	OG1	THR	58	-3 403
1 313	-11 862	1 00	0.00	BrD ATOM	957	HG1	THR	58	-3 101
1 133	-12 755	1 00	0 00	BrD ATOM	958	CG2	THR	58	-1 197
2 099	-11 525	1.00	0.00	BrD ATOM	959	HG21	THR	58	-0.808
2 734	-10 743	1 00	0.00	BrD ATOM	960	HG22	THR	58	-1 585
2 710	-12 326	1 00	0 00	BrD ATOM	961	HG23	THR	58	-0 405
1 469	-11.904	1.00	0.00	BrD ATOM	962	C	THR	58	-0 539
0 305	-10 045	1 00	0 00	BrD ATOM	963	O	THR	58	0 499
0 220	-10 701	1 00	0 00	BrD ATOM	964	N	MET	59	-0 537
0.445	-8 721	1.00	0 00	BrD ATOM	965	HN	MET	59	-1 388
0 503	-8 238	1.00	0.00	BrD ATOM	966	CA	MET	59	0 718
0 505	-7 972	1 00	0.00	BrD ATOM	967	HA	MET	59	1 401
0 191	-8 436	1 00	0 00	BrD ATOM	968	CB	MET	59	0.499
0 070	-6 513	1.00	0 00	BrD ATOM	969	HB1	MET	59	1.430
0 316	-6 125	1.00	0 00	BrD ATOM	970	HB2	MET	59	-0 238
0 717	-6.498	1 00	0 00	BrD ATOM	971	CG	MET	59	0.022
1 176	-5.583	1 00	0 00	BrD ATOM	972	HG1	MET	59	-0 822
0 811	-5 017	1 00	0 00	BrD ATOM	973	HG2	MET	59	-0.286
2 022	-6 180	1 00	0.00	BrD ATOM	974	SD	MET	59	1 300
1.715	-4 431	1.00	0.00	BrD ATOM	975	CE	MET	59	1 463
0 259	-3 400	1 00	0.00	BrD ATOM	976	HE1	MET	59	0 629
0 205	-2 715	1 00	0 00	BrD ATOM	977	HE2	MET	59	1 474
0 624	-4 022	1.00	0 00	BrD ATOM	978	HE3	MET	59	2.386
0 316	-2 841	1 00	0.00	BrD ATOM	979	C	MET	59	1 345
1 901	-8 036	1 00	0 00	BrD ATOM	980	O	MET	59	2.535
2 067	-7 767	1 00	0.00	BrD ATOM	981	N	SER	60	0.542
2.898	-8 392	1 00	0 00	BrD ATOM	982	HN	SER	60	-0.399
2 710	-8.590	1 00	0 00	BrD ATOM	983	CA	SER	60	1 025
4.271	-8 478	1.00	0 00	BrD ATOM	984	HA	SER	60	1 685
4 442	-7 640	1 00	0 00	BrD ATOM	985	CB	SER	60	-0.147
5 250	-8.396	1 00	0.00	BrD ATOM	986	HB1	SER	60	-0.610
5.171	-7 424	1 00	0.00	BrD ATOM	987	HB2	SER	60	-0.871
5.006	-9.159	1 00	0.00	BrD ATOM	988	OG	SER	60	0 286
6 585	-8 588	1.00	0 00	BrD ATOM	989	HG	SER	60	-0 145
6 953	-9.363	1 00	0 00	BrD ATOM	990	C	SER	60	1 803
4 503	-9 770	1.00	0 00	BrD ATOM	991	O	SER	60	2 636
5.405	-9 850	1 00	0 00	BrD ATOM	992	N	GLU	61	1.519
3 690	-10 782	1 00	0 00	BrD ATOM	993	HN	GLU	61	0.839
2 995	-10 661	1 00	0.00	BrD ATOM	994	CA	GLU	61	2 182
3 820	-12 075	1 00	0 00	BrD ATOM	995	HA	GLU	61	2 295
4 874	-12 283	1.00	0 00	BrD ATOM	996	CB	GLU	61	1 326
3.187	-13 174	1.00	0 00	BrD ATOM	997	HB1	GLU	61	1.820
3 324	-14 125	1.00	0 00	BrD ATOM	998	HB2	GLU	61	1 232
2 129	-12.977	1 00	0.00	BrD ATOM	999	CG	GLU	61	-0 071
3 779	-13 274	1 00	0 00	BrD ATOM	1000	HG1	GLU	61	-0 494
3 836	-12.282	1 00	0 00	BrD ATOM	1001	HG2	GLU	61	-0 679
3.132	-13 889	1 00	0 00	BrD ATOM	1002	CD	GLU	61	-0.073
5 167	-13 883	1 00	0 00	BrD ATOM	1003	OE1	GLU	61	-1.024
5 488	-14 627	1.00	0 00	BrD ATOM	1004	OE2	GLU	61	0.876
5.934	-13.617	1.00	0.00	BrD ATOM	1005	C	GLU	61	3.565
3.174	-12.060	1.00	0.00	BrD ATOM	1006	O	GLU	61	4.466
3 601	-12 782	1.00	0.00	BrD ATOM	1007	N	ARG	62	3 726
2.137	-11.244	1 00	0 00	BrD ATOM	1008	HN	ARG	62	2 971
1 836	-10.697	1 00	0 00	BrD ATOM	1009	CA	ARG	62	4 999
1.428	-11.155	1 00	0 00	BrD ATOM	1010	HA	ARG	62	5 352
1 262	-12 162	1.00	0 00	BrD ATOM	1011	CB	ARG	62	4 807
0.075	-10.468	1.00	0 00	BrD ATOM	1012	HB1	ARG	62	5 753
0.241	-10 052	1 00	0.00	BrD ATOM	1013	HB2	ARG	62	4 091
0.187	-9 668	1 00	0 00	BrD ATOM	1014	CG	ARG	62	4 312
1.018	-11.404	1 00	0 00	BrD ATOM	1015	HG1	ARG	62	4 852
1.928	-11 195	1 00	0.00	BrD ATOM	1016	HG2	ARG	62	4.494
0.714	-12 424	1 00	0.00	BrD ATOM	1017	CD	ARG	62	2 826
1 278	-11 225	1.00	0 00	BrD ATOM	1018	HD1	ARG	62	2 484
0.738	-10.356	1.00	0 00	BrD ATOM	1019	HD2	ARG	62	2 675
2 336	-11 072	1.00	0 00	BrD ATOM	1020	NE	ARG	62	2 052
0.851	-12 387	1.00	0 00	BrD ATOM	1021	HE	ARG	62	1 621
0 028	-12 346	1 00	0 00	BrD ATOM	1022	CZ	ARG	62	1 903
1.585	-13 485	1 00	0 00	BrD ATOM	1023	NH1	ARG	62	1 183
1 125	-14 498	1 00	0.00	BrD ATOM	1024	HH11	ARG	62	1 072
1 678	-15 324	1 00	0.00	BrD ATOM	1025	HH12	ARG	62	0 752
0.226	-14.437	1 00	0.00	BrD ATOM	1026	NH2	ARG	62	2 473
2.780	-13.571	1.00	0.00	BrD ATOM	1027	HH21	ARG	62	2 359
3 329	-14.399	1 00	0 00	BrD ATOM	1028	HH22	ARG	62	3 018
3 130	-12 809	1 00	0 00	BrD ATOM	1029	C	ARG	62	6 040
2 255	-10 405	1 00	0 00	BrD ATOM	1030	O	ARG	62	7 101
2 569	-10 945	1 00	0 00	BrD ATOM	1031	N	LEU	63	5 734
2 606	-9 158	1.00	0 00	BrD ATOM	1032	HN	LEU	63	4 875
2 326	-8 780	1 00	0 00	BrD ATOM	1033	CA	LEU	63	6 651
3.396	-8.339	1.00	0 00	BrD ATOM	1034	HA	LEU	63	7.496
2.771	-8 093	1.00	0 00	BrD ATOM	1035	CB	LEU	63	5 962
3 840	-7 043	1 00	0 00	BrD ATOM	1036	HB1	LEU	63	5 009
4 277	-7 302	1 00	0 00	BrD ATOM	1037	HB2	LEU	63	5 780
2 962	-6 442	1 00	0 00	BrD ATOM	1038	CG	LEU	63	6 736
4 857	-6 186	1 00	0 00	BrD ATOM	1039	HG	LEU	63	6 429
4 754	-5 156	1.00	0.00	BrD ATOM	1040	CD1	LEU	63	8 237
4.605	-6 247	1.00	0.00	BrD ATOM	1041	HD11	LEU	63	8 420
3 584	-6 547	1.00	0 00	BrD ATOM	1042	HD12	LEU	63	8 685
5.277	-6 965	1 00	0 00	BrD ATOM	1043	HD13	LEU	63	8 671
4.779	-5 273	1 00	0 00	BrD ATOM	1044	CD2	LEU	63	6 414
6.277	-6 627	1 00	0 00	BrD ATOM	1045	HD21	LEU	63	7 332
6 804	-6 842	1 00	0.00	BrD ATOM	1046	HD22	LEU	63	5 798
6 248	-7 514	1 00	0 00	BrD ATOM	1047	HD23	LEU	63	5 883
6 787	-5 836	1 00	0 00	BrD ATOM	1048	C	LEU	63	7 150
4 618	-9 103	1 00	0 00	BrD ATOM	1049	O	LEU	63	8 354
4 853	-9.203	1 00	0.00	BrD ATOM	1050	N	LYS	64	6 214
5 390	-9 643	1.00	0 00	BrD ATOM	1051	HN	LYS	64	5 271
5 150	-9 525	1.00	0 00	BrD ATOM	1052	CA	LYS	64	6 551
6 592	-10 397	1 00	0.00	BrD ATOM	1053	HA	LYS	64	6 929
7.325	-9 699	1 00	0.00	BrD ATOM	1054	CB	LYS	64	5 303
7 152	-11 082	1.00	0 00	BrD ATOM	1055	HB1	LYS	64	4 649
6 332	-11.340	1 00	0 00	BrD ATOM	1056	HB2	LYS	64	5 602
7 661	-11.987	1 00	0 00	BrD ATOM	1057	CG	LYS	64	4 523
8 131	-10 221	1.00	0 00	BrD ATOM	1058	HG1	LYS	64	3 533
7 734	-10 047	1 00	0.00	BrD ATOM	1059	HG2	LYS	64	5 035
8.254	-9.278	1.00	0 00	BrD ATOM	1060	CD	LYS	64	4.398
9 488	-10 894	1 00	0 00	BrD ATOM	1061	HD1	LYS	64	3 363
9.798	-10 870	1 00	0 00	BrD ATOM	1062	HD2	LYS	64	4 726
9 402	-11 920	1 00	0 00	BrD ATOM	1063	CE	LYS	64	5 243
10 538	-10 192	1.00	0.00	BrD ATOM	1064	HE1	LYS	64	5 904
10 043	-9.496	1 00	0.00	BrD ATOM	1065	HE2	LYS	64	4.589
11 207	-9 653	1.00	0 00	BrD ATOM	1066	NZ	LYS	64	6.060
11 330	-11 154	1.00	0.00	BrD ATOM	1067	HZ1	LYS	64	6.712
11.955	-10.638	1.00	0 00	BrD ATOM	1068	HZ2	LYS	64	6 615
10.693	-11.761	1.00	0 00	BrD ATOM	1069	HZ3	LYS	64	5.441
11 911	-11 754	1 00	0 00	BrD ATOM	1070	C	LYS	64	7 629
6.305	-11 439	1.00	0 00	BrD ATOM	1071	O	LYS	64	8 376
7 200	-11 834	1 00	0 00	BrD ATOM	1072	N	ASN	65	7.705
5 052	-11 880	1 00	0.00	BrD ATOM	1073	HN	ASN	65	7.080
4 383	-11 531	1 00	0.00	BrD ATOM	1074	CA	ASN	65	8 688
4 657	-12 883	1 00	0 00	BrD ATOM	1075	HA	ASN	65	9 212
5 547	-13 198	1 00	0.00	BrD ATOM	1076	CB	ASN	65	7 989
4 034	-14.092	1 00	0 00	BrD ATOM	1077	HB1	ASN	65	8 680
3 376	-14.600	1.00	0.00	BrD ATOM	1078	HB2	ASN	65	7 137
3.463	-13 754	1.00	0 00	BrD ATOM	1079	CG	ASN	65	7 506
5 076	-15.081	1.00	0 00	BrD ATOM	1080	OD1	ASN	65	8 177
6.080	-15.320	1 00	0 00	BrD ATOM	1081	ND2	ASN	65	6 334
4.844	-15 660	1 00	0 00	BrD ATOM	1082	HD21	ASN	65	5 854
4.024	-15 421	1.00	0 00	BrD ATOM	1083	HD22	ASN	65	5 997
5 502	-16 303	1 00	0.00	BrD ATOM	1084	C	ASN	65	9 703
3 677	-12.308	1 00	0.00	BrD ATOM	1085	O	ASN	65	10 237
2.829	-13 023	1 00	0.00	BrD ATOM	1086	N	ARG	66	9 973
3 804	-11.014	1.00	0 00	BrD ATOM	1087	HN	ARG	66	9 523
4.505	-10.498	1.00	0 00	BrD ATOM	1088	CA	ARG	66	10 942
2.943	-10 346	1 00	0 00	BrD ATOM	1089	HA	ARG	66	10 826
3.082	-9 281	1 00	0.00	BrD ATOM	1090	CB	ARG	66	12 357
3.347	-10 739	1 00	0.00	BrD ATOM	1091	HB1	ARG	66	12 323
3.875	-11 680	1.00	0 00	BrD ATOM	1092	HB2	ARG	66	12.959
2 458	-10.854	1.00	0 00	BrD ATOM	1093	CG	ARG	66	13.018
4.243	-9 713	1.00	0 00	BrD ATOM	1094	HG1	ARG	66	13.744
3.666	-9.163	1.00	0.00	BrD ATOM	1095	HG2	ARG	66	12 262
4.613	-9.038	1 00	0.00	BrD ATOM	1096	CD	ARG	66	13.710
5 423	-10 368	1 00	0 00	BrD ATOM	1097	HD1	ARG	66	13.453
5 439	-11 416	1 00	0 00	BrD ATOM	1098	HD2	ARG	66	13.358

6 329	-9 898	1 00	0.00	BrD ATOM	1099	NE	ARG	66	15 162
5 351	-10 237	1 00	0 00	BrD ATOM	1100	HE	ARG	66	15 688
5 255	-11 059	1.00	0 00	BrD ATOM	1101	CZ	ARG	66	15 801
5 407	-9 074	1 00	0 00	BrD ATOM	1102	NH1	ARG	66	15.117
5.536	-7 945	1.00	0 00	BrD ATOM	1103	HH11	ARG	66	15.599
5 578	-7 070	1 00	0 00	BrD ATOM	1104	HH12	ARG	66	14 118
5 591	-7 969	1 00	0 00	BrD ATOM	1105	NH2	ARG	66	17.125
5 334	-9 037	1 00	0 00	BrD ATOM	1106	HH21	ARG	66	17 604
5 377	-8 161	1 00	0.00	BrD ATOM	1107	HH22	ARG	66	17 643
5.237	-9.887	1.00	0 00	BrD ATOM	1108	C	ARG	66	10 708
1 474	-10 682	1 00	0 00	BrD ATOM	1109	O	ARG	66	11 654
0 705	-10.850	1 00	0 00	BrD ATOM	1110	N	TYR	67	9 441
1 097	-10 783	1 00	0 00	BrD ATOM	1111	HN	TYR	67	8 736
1.759	-10 633	1 00	0 00	BrD ATOM	1112	CA	TYR	67	9 075
0.280	-11 094	1 00	0 00	BrD ATOM	1113	HA	TYR	67	9 952
0 780	-11 472	1 00	0.00	BrD ATOM	1114	CB	TYR	67	7 982
0 309	-12 164	1 00	0 00	BrD ATOM	1115	HB1	TYR	67	7 062
0 061	-11 738	1 00	0 00	BrD ATOM	1116	HB2	TYR	67	8 276
0 330	-12 984	1 00	0 00	BrD ATOM	1117	CG	TYR	67	7 713
1 687	-12 723	1.00	0 00	BrD ATOM	1118	CD1	TYR	67	7 042
2.639	-11 970	1.00	0 00	BrD ATOM	1119	HD1	TYR	67	6 718
2 385	-10 973	1 00	0 00	BrD ATOM	1120	CD2	TYR	67	8 122
2 032	-14 005	1 00	0.00	BrD ATOM	1121	HD2	TYR	67	8 645
1 301	-14 604	1 00	0 00	BrD ATOM	1122	CE1	TYR	67	6 787
3.899	-12 475	1 00	0 00	BrD ATOM	1123	HE1	TYR	67	6 261
4 625	-11 872	1 00	0 00	BrD ATOM	1124	CE2	TYR	67	7 872
3 291	-14 518	1 00	0 00	BrD ATOM	1125	HE2	TYR	67	8 198
3 541	-15 516	1 00	0 00	BrD ATOM	1126	CZ	TYR	67	7.204
4.220	-13 749	1 00	0 00	BrD ATOM	1127	OH	TYR	67	6.953
5 475	-14 256	1 00	0.00	BrD ATOM	1128	HH	TYR	67	7 446
6.127	-13 753	1.00	0 00	BrD ATOM	1129	C	TYR	67	8 606
1 006	-9 840	1 00	0.00	BrD ATOM	1130	O	TYR	67	8.910
2 181	-9 639	1 00	0 00	BrD ATOM	1131	N	TYR	68	7 880
0.291	-8 990	1.00	0 00	BrD ATOM	1132	HN	TYR	68	7.686
0 647	-9 197	1 00	0 00	BrD ATOM	1133	CA	TYR	68	7.401
0 855	-7 736	1 00	0 00	BrD ATOM	1134	HA	TYR	68	7.528
1 924	-7 788	1 00	0 00	BrD ATOM	1135	CB	TYR	68	5 918
0 531	-7 538	1.00	0.00	BrD ATOM	1136	HB1	TYR	68	5 646
0.286	-8 188	1 00	0 00	BrD ATOM	1137	HB2	TYR	68	5 758
0.234	-6 512	1 00	0 00	BrD ATOM	1138	CG	TYR	68	4 987
1 689	-7 833	1.00	0 00	BrD ATOM	1139	CD1	TYR	68	5 378
2 734	-8 664	1 00	0 00	BrD ATOM	1140	HD1	TYR	68	6 364
2 717	-9 101	1 00	0 00	BrD ATOM	1141	CD2	TYR	68	3 712
1.732	-7.283	1.00	0 00	BrD ATOM	1142	HD2	TYR	68	3 392
0 927	-6 638	1 00	0 00	BrD ATOM	1143	CE1	TYR	68	4.526
3 788	-8 933	1 00	0 00	BrD ATOM	1144	HE1	TYR	68	4 849
4 591	-9 579	1.00	0 00	BrD ATOM	1145	CE2	TYR	68	2 855
2 782	-7 549	1 00	0 00	BrD ATOM	1146	HE2	TYR	68	1 868
2 797	-7 110	1 00	0 00	BrD ATOM	1147	CZ	TYR	68	3 267
3 807	-8 374	1 00	0.00	BrD ATOM	1148	OH	TYR	68	2 416
4 855	-8 639	1 00	0 00	BrD ATOM	1149	HH	TYR	68	2 457
5 490	-7 920	1 00	0 00	BrD ATOM	1150	C	TYR	68	8 206
0 327	-6 548	1 00	0 00	BrD ATOM	1151	O	TYR	68	8 001
0 759	-5 416	1.00	0 00	BrD ATOM	1152	N	VAL	69	9 149
0.579	-6 816	1.00	0 00	BrD ATOM	1153	HN	VAL	69	9.268
0.888	-7 735	1 00	0.00	BrD ATOM	1154	CA	VAL	69	9 977
1.170	-5 769	1 00	0 00	BrD ATOM	1155	HA	VAL	69	9 397
1.941	-5 285	1 00	0 00	BrD ATOM	1156	CB	VAL	69	11.232
1 825	-6 366	1 00	0 00	BrD ATOM	1157	HB	VAL	69	10.922
2.537	-7 117	1.00	0.00	BrD ATOM	1158	CG1	VAL	69	12 107
0 778	-7 032	1 00	0 00	BrD ATOM	1159	HG11	VAL	69	11 701
0.536	-8 003	1.00	0 00	BrD ATOM	1160	HG12	VAL	69	13.108
1 165	-7 146	1 00	0 00	BrD ATOM	1161	HG13	VAL	69	12 131
0 111	-6 420	1 00	0.00	BrD ATOM	1162	CG2	VAL	69	12 001
2.572	-5 291	1 00	0 00	BrD ATOM	1163	HG21	VAL	69	11 389
3 370	-4 899	1.00	0 00	BrD ATOM	1164	HG22	VAL	69	12.256
1 889	-4 494	1 00	0 00	BrD ATOM	1165	HG23	VAL	69	12 904
2.985	-5 716	1 00	0 00	BrD ATOM	1166	C	VAL	69	10 409
0 149	-4 717	1.00	0 00	BrD ATOM	1167	O	VAL	69	10 642
0 506	-3 565	1.00	0 00	BrD ATOM	1168	N	SER	70	10 508
1 123	-5 110	1 00	0.00	BrD ATOM	1169	HN	SER	70	10.321
1.350	-6.044	1.00	0 00	BrD ATOM	1170	CA	SER	70	10 909
2 190	-4 189	1 00	0.00	BrD ATOM	1171	HA	SER	70	11 983
2 146	-4 081	1 00	0 00	BrD ATOM	1172	CB	SER	70	10 525
3 552	-4 767	1 00	0 00	BrD ATOM	1173	HB1	SER	70	11.246
3.838	-5.518	1.00	0 00	BrD ATOM	1174	HB2	SER	70	9.546
3 483	-5.216	1 00	0 00	BrD ATOM	1175	OG	SER	70	10 498
4.547	-3 758	1 00	0.00	BrD ATOM	1176	HG	SER	70	10 908
5 349	-4.088	1 00	0 00	BrD ATOM	1177	C	SER	70	10 268
2 011	-2 810	1 00	0 00	BrD ATOM	1178	O	SER	70	9 252
1 330	-2 674	1 00	0.00	BrD ATOM	1179	N	LYS	71	10 881
2 605	-1 791	1.00	0 00	BrD ATOM	1180	HN	LYS	71	11 700
3 118	-1.958	1.00	0 00	BrD ATOM	1181	CA	LYS	71	10 393
2.470	-0 422	1 00	0 00	BrD ATOM	1182	HA	LYS	71	10.268
1.415	-0.226	1 00	0.00	BrD ATOM	1183	CB	LYS	71	11 419
3 036	0 564	1.00	0.00	BrD ATOM	1184	HB1	LYS	71	10 915
3 287	1 485	1 00	0.00	BrD ATOM	1185	HB2	LYS	71	11 848
3.933	0.142	1.00	0 00	BrD ATOM	1186	CG	LYS	71	12.550
2.074	0 888	1 00	0.00	BrD ATOM	1187	HG1	LYS	71	13.359
2 237	0 191	1.00	0 00	BrD ATOM	1188	HG2	LYS	71	12 188
1 061	0.791	1.00	0 00	BrD ATOM	1189	CD	LYS	71	13 069
2 279	2 302	1 00	0 00	BrD ATOM	1190	HD1	LYS	71	12.295
2 001	3 002	1 00	0.00	BrD ATOM	1191	HD2	LYS	71	13 936
1 652	2 452	1 00	0.00	BrD ATOM	1192	CE	LYS	71	13 460

3.727	2.548	1.00	0.00	BrD ATOM	1193	HE1	LYS	71	14.024
4.084	1 699	1 00	0.00	BrD ATOM	1194	HE2	LYS	71	12.561
4 316	2.655	1.00	0.00	BrD ATOM	1195	NZ	LYS	71	14 287
3 879	3 777	1.00	0 00	BrD ATOM	1196	HZ1	LYS	71	13 870
3 334	4 558	1 00	0.00	BrD ATOM	1197	HZ2	LYS	71	14.334
4 880	4 055	1.00	0.00	BrD ATOM	1198	HZ3	LYS	71	15 252
3 533	3 604	1.00	0.00	BrD ATOM	1199	C	LYS	71	9 041
3.160	-0 231	1 00	0 00	BrD ATOM	1200	O	LYS	71	7 992
2.529	-0.362	1 00	0 00	BrD ATOM	1201	N	LYS	72	9 070
4 447	0 109	1.00	0.00	BrD ATOM	1202	HN	LYS	72	9 933
4 898	0.211	1 00	0.00	BrD ATOM	1203	CA	LYS	72	7 844
5.201	0 351	1 00	0.00	BrD ATOM	1204	HA	LYS	72	7 396
4 818	1 255	1 00	0 00	BrD ATOM	1205	CB	LYS	72	8.167
6 684	0.547	1 00	0 00	BrD ATOM	1206	HB1	LYS	72	7 249
7 216	0 752	1 00	0 00	BrD ATOM	1207	HB2	LYS	72	8 601
7 070	-0 364	1.00	0 00	BrD ATOM	1208	CG	LYS	72	9 136
6 950	1 687	1 00	0 00	BrD ATOM	1209	HG1	LYS	72	9 870
6.158	1 715	1 00	0.00	BrD ATOM	1210	HG2	LYS	72	9 629
7 895	1.515	1.00	0.00	BrD ATOM	1211	CD	LYS	72	8 419
7 004	3 027	1.00	0 00	BrD ATOM	1212	HD1	LYS	72	7 833
6.104	3 147	1 00	0 00	BrD ATOM	1213	HD2	LYS	72	9.155
7 065	3 816	1 00	0.00	BrD ATOM	1214	CE	LYS	72	7 497
8 208	3.117	1.00	0.00	BrD ATOM	1215	HE1	LYS	72	7.708
8.869	2 288	1 00	0 00	BrD ATOM	1216	HE2	LYS	72	6 474
7.868	3 054	1 00	0 00	BrD ATOM	1217	NZ	LYS	72	7 681
8 956	4.391	1 00	0.00	BrD ATOM	1218	HZ1	LYS	72	8 150
8 352	5 096	1.00	0 00	BrD ATOM	1219	HZ2	LYS	72	6 758
9 256	4 766	1 00	0 00	BrD ATOM	1220	HZ3	LYS	72	8.267
9 800	4.229	1 00	0 00	BrD ATOM	1221	C	LYS	72	6 852
5 034	-0 794	1.00	0 00	BrD ATOM	1222	O	LYS	72	5 641
5.001	-0 578	1.00	0.00	BrD ATOM	1223	N	LEU	73	7 370
4 933	-2 011	1 00	0 00	BrD ATOM	1224	HN	LEU	73	8 343
4 972	-2 121	1.00	0.00	BrD ATOM	1225	CA	LEU	73	6.528
4 786	-3 191	1.00	0.00	BrD ATOM	1226	HA	LEU	73	5.982
5 708	-3 323	1 00	0 00	BrD ATOM	1227	CB	LEU	73	7.394
4.539	-4 427	1 00	0 00	BrD ATOM	1228	HB1	LEU	73	7 447
3 474	-4 596	1 00	0.00	BrD ATOM	1229	HB2	LEU	73	8 389
4 903	-4.219	1.00	0.00	BrD ATOM	1230	CG	LEU	73	6 896
5 206	-5 711	1.00	0.00	BrD ATOM	1231	HG	LEU	73	5.937
4.787	-5 978	1 00	0 00	BrD ATOM	1232	CD1	LEU	73	7 860
4 943	-6 857	1 00	0 00	BrD ATOM	1233	HD11	LEU	73	8 166
3 907	-6.840	1 00	0 00	BrD ATOM	1234	HD12	LEU	73	8 729
5 576	-6.750	1 00	0 00	BrD ATOM	1235	HD13	LEU	73	7 372
5 158	-7 796	1.00	0 00	BrD ATOM	1236	CD2	LEU	73	6.710
6.701	-5 498	1 00	0 00	BrD ATOM	1237	HD21	LEU	73	7 104
6.979	-4 531	1 00	0 00	BrD ATOM	1238	HD22	LEU	73	5 659
6 943	-5 541	1 00	0 00	BrD ATOM	1239	HD23	LEU	73	7 237
7 243	-6 270	1.00	0.00	BrD ATOM	1240	C	LEU	73	5 528
3 645	-3.025	1.00	0.00	BrD ATOM	1241	O	LEU	73	4.318
3.860	-3 061	1 00	0 00	BrD ATOM	1242	N	PHE	74	6 041
2 432	-2 860	1 00	0.00	BrD ATOM	1243	HN	PHE	74	7.014
2 322	-2 855	1 00	0 00	BrD ATOM	1244	CA	PHE	74	5 192
1.253	-2 721	1 00	0 00	BrD ATOM	1245	HA	PHE	74	4.364
1.359	-3 406	1 00	0 00	BrD ATOM	1246	CB	PHE	74	5 984
0 003	-3 084	1.00	0 00	BrD ATOM	1247	HB1	PHE	74	6 730
0 181	-2.324	1.00	0.00	BrD ATOM	1248	HB2	PHE	74	6 473
0 154	-4 030	1 00	0 00	BrD ATOM	1249	CG	PHE	74	5 141
1.240	-3 202	1 00	0 00	BrD ATOM	1250	CD1	PHE	74	4 952
1 851	-4 431	1.00	0.00	BrD ATOM	1251	HD1	PHE	74	5 412
1 425	-5 311	1 00	0.00	BrD ATOM	1252	CD2	PHE	74	4.546
1.797	-2 082	1 00	0 00	BrD ATOM	1253	HD2	PHE	74	4.691
1 332	-1.118	1 00	0 00	BrD ATOM	1254	CE1	PHE	74	4 181
2 993	-4.542	1.00	0.00	BrD ATOM	1255	HE1	PHE	74	4 039
3 458	-5.506	1 00	0.00	BrD ATOM	1256	CE2	PHE	74	3 780
2.942	-2 186	1 00	0 00	BrD ATOM	1257	HE2	PHE	74	3 315
3 362	-1 304	1.00	0 00	BrD ATOM	1258	CZ	PHE	74	3 593
3 538	-3 418	1.00	0.00	BrD ATOM	1259	HZ	PHE	74	2.989
4 430	-3.502	1.00	0 00	BrD ATOM	1260	C	PHE	74	4 643
1 116	-1 305	1 00	0 00	BrD ATOM	1261	O	PHE	74	3.503
0.694	-1 111	1 00	0 00	BrD ATOM	1262	N	MET	75	5 466
1 447	-0 318	1 00	0 00	BrD ATOM	1263	HN	MET	75	6.372
1 755	-0.532	1 00	0.00	BrD ATOM	1264	CA	MET	75	5 072
1.308	1.078	1 00	0.00	BrD ATOM	1265	HA	MET	75	4 603
0.339	1 187	1 00	0 00	BrD ATOM	1266	CB	MET	75	6.300
1 365	1 984	1 00	0 00	BrD ATOM	1267	HB1	MET	75	6 001
1 734	2 954	1 00	0 00	BrD ATOM	1268	HB2	MET	75	7 021
2.043	1 554	1.00	0.00	BrD ATOM	1269	CG	MET	75	6 966
0.014	2 171	1 00	0 00	BrD ATOM	1270	HG1	MET	75	7.524
0 029	3 092	1 00	0 00	BrD ATOM	1271	HG2	MET	75	6.200
0 744	2.231	1.00	0 00	BrD ATOM	1272	SD	MET	75	8 086
0 403	0.822	1.00	0.00	BrD ATOM	1273	CE	MET	75	8 173
2 182	1 002	1.00	0 00	BrD ATOM	1274	HE1	MET	75	7 211
2 557	1.319	1.00	0 00	BrD ATOM	1275	HE2	MET	75	8 917
2 435	1.741	1.00	0 00	BrD ATOM	1276	HE3	MET	75	8 438
2 630	0.054	1.00	0.00	BrD ATOM	1277	C	MET	75	4.067
2.374	1 496	1 00	0.00	BrD ATOM	1278	O	MET	75	2.939
2 052	1.866	1 00	0 00	BrD ATOM	1279	N	ALA	76	4 472
3.642	1 462	1.00	0 00	BrD ATOM	1280	HN	ALA	76	5 380
3 854	1 163	1.00	0.00	BrD ATOM	1281	CA	ALA	76	3.573
4 722	1 861	1.00	0 00	BrD ATOM	1282	HA	ALA	76	3.409
4.638	2 922	1 00	0 00	BrD ATOM	1283	CB	ALA	76	4 182
6.083	1.595	1 00	0.00	BrD ATOM	1284	HB1	ALA	76	4 234
6 252	0 531	1.00	0.00	BrD ATOM	1285	HB2	ALA	76	5 172
6 125	2.021	1 00	0 00	BrD ATOM	1286	HB3	ALA	76	3 558

6.842	2.049	1.00	0.00	BrD ATOM	1287	C	ALA	76	2.240
4.601	1 147	1 00	0 00	BrD ATOM	1288	O	ALA	76	1.211
5.026	1 666	1 00	0.00	BrD ATOM	1289	N	ASP	77	2.270
4.014	-0 044	1 00	0.00	BrD ATOM	1290	HN	ASP	77	3 124
3.685	-0.394	1 00	0 00	BrD ATOM	1291	CA	ASP	77	1 058
3 804	-0 818	1.00	0.00	BrD ATOM	1292	HA	ASP	77	0 460
4 701	-0 750	1.00	0 00	BrD ATOM	1293	CB	ASP	77	1.392
3.534	-2.283	1 00	0 00	BrD ATOM	1294	HB1	ASP	77	2 196
2.817	-2 334	1 00	0 00	BrD ATOM	1295	HB2	ASP	77	0.521
3 128	-2 776	1 00	0 00	BrD ATOM	1296	CG	ASP	77	1 817
4 790	-3.018	1.00	0.00	BrD ATOM	1297	OD1	ASP	77	1.353
4.995	-4 159	1.00	0 00	BrD ATOM	1298	OD2	ASP	77	2.613
5.569	-2.453	1 00	0 00	BrD ATOM	1299	C	ASP	77	0 268
2.641	-0 243	1.00	0.00	BrD ATOM	1300	O	ASP	77	-0 950
2 717	-0 113	1.00	0.00	BrD ATOM	1301	N	LEU	78	0 970
1.569	0 119	1 00	0 00	BrD ATOM	1302	HN	LEU	78	1.944
1.570	0 006	1 00	0 00	BrD ATOM	1303	CA	LEU	78	0 319
0 411	0 711	1 00	0 00	BrD ATOM	1304	HA	LEU	78	-0 493
0 122	0.060	1 00	0 00	BrD ATOM	1305	CB	LEU	78	1 280
0 761	0 849	1 00	0 00	BrD ATOM	1306	HB1	LEU	78	2 212
0 516	0 358	1 00	0 00	BrD ATOM	1307	HB2	LEU	78	1 480
0 922	1 900	1.00	0 00	BrD ATOM	1308	CG	LEU	78	0 736
2.052	0.259	1.00	0 00	BrD ATOM	1309	HG	LEU	78	-0 338
2.023	0 293	1 00	0.00	BrD ATOM	1310	CD1	LEU	78	1 143
2 189	-1 193	1.00	0 00	BrD ATOM	1311	HD11	LEU	78	1 413
3.213	-1 398	1 00	0 00	BrD ATOM	1312	HD12	LEU	78	1 985
1 543	-1 388	1 00	0 00	BrD ATOM	1313	HD13	LEU	78	0 317
1.901	-1 825	1 00	0 00	BrD ATOM	1314	CD2	LEU	78	1 189
3 236	1 078	1 00	0.00	BrD ATOM	1315	HD21	LEU	78	2.264
3 266	1 099	1 00	0 00	BrD ATOM	1316	HD22	LEU	78	0 808
4.145	0.640	1 00	0.00	BrD ATOM	1317	HD23	LEU	78	0 809
3.130	2 084	1 00	0.00	BrD ATOM	1318	C	LEU	78	-0 253
0 769	2.066	1 00	0 00	BrD ATOM	1319	O	LEU	78	-1 459
0 663	2 292	1 00	0 00	BrD ATOM	1320	N	GLN	79	0 611
1 252	2 952	1 00	0.00	BrD ATOM	1321	HN	GLN	79	1 551
1 353	2 700	1 00	0 00	BrD ATOM	1322	CA	GLN	79	0 171
1 723	4 254	1.00	0.00	BrD ATOM	1323	HA	GLN	79	-0 198
0.873	4 807	1 00	0.00	BrD ATOM	1324	CB	GLN	79	1 338
2 361	5 015	1 00	0.00	BrD ATOM	1325	HB1	GLN	79	1 045
2 520	6 038	1 00	0 00	BrD ATOM	1326	HB2	GLN	79	2 180
1 686	4 991	1 00	0.00	BrD ATOM	1327	CG	GLN	79	1 781
3 694	4 448	1 00	0 00	BrD ATOM	1328	HG1	GLN	79	1 501
3.740	3 407	1 00	0 00	BrD ATOM	1329	HG2	GLN	79	2 855
3 766	4 538	1 00	0 00	BrD ATOM	1330	CD	GLN	79	1 158
4.871	5 172	1 00	0.00	BrD ATOM	1331	OE1	GLN	79	0 409
5.651	4 585	1 00	0 00	BrD ATOM	1332	NE2	GLN	79	1 467
5 005	6.457	1.00	0 00	BrD ATOM	1333	HE21	GLN	79	1.079
5 757	6 950	1 00	0 00	BrD ATOM	1334	HE22	GLN	79	2 070
4 346	6 859	1 00	0 00	BrD ATOM	1335	C	GLN	79	-0 960
2 732	4.074	1.00	0.00	BrD ATOM	1336	O	GLN	79	-1 787
2.924	4 964	1 00	0 00	BrD ATOM	1337	N	ARG	80	-0.997
3 356	2 895	1 00	0 00	BrD ATOM	1338	HN	ARG	80	-0.321
3 140	2 216	1 00	0 00	BrD ATOM	1339	CA	ARG	80	-2 048
4.306	2 560	1.00	0 00	BrD ATOM	1340	HA	ARG	80	-2 275
4.880	3 447	1.00	0 00	BrD ATOM	1341	CB	ARG	80	-1 579
5 253	1 451	1 00	0.00	BrD ATOM	1342	HB1	ARG	80	-2 401
5 429	0 773	1.00	0.00	BrD ATOM	1343	HB2	ARG	80	-0 770
4 785	0.908	1.00	0 00	BrD ATOM	1344	CG	ARG	80	-1 092
6 598	1.964	1 00	0.00	BrD ATOM	1345	HG1	ARG	80	-0 290
6 434	2 669	1.00	0.00	BrD ATOM	1346	HG2	ARG	80	-0.728
7 180	1 131	1.00	0 00	BrD ATOM	1347	CD	ARG	80	-2 206
7.367	2.654	1.00	0 00	BrD ATOM	1348	HD1	ARG	80	-3 054
6 711	2 780	1 00	0 00	BrD ATOM	1349	HD2	ARG	80	-2 486
8 203	2 031	1 00	0.00	BrD ATOM	1350	NE	ARG	80	-1 796
7 867	3 962	1 00	0.00	BrD ATOM	1351	HE	ARG	80	-0 837
7 874	4 166	1.00	0.00	BrD ATOM	1352	CZ	ARG	80	-2.648
8.310	4 881	1 00	0.00	BrD ATOM	1353	NH1	ARG	80	-2 198
8 750	6 047	1 00	0.00	BrD ATOM	1354	HH11	ARG	80	-1 216
8 749	6 237	1 00	0.00	BrD ATOM	1355	HH12	ARG	80	-2 840
9.083	6.738	1.00	0 00	BrD ATOM	1356	NH2	ARG	80	-3 950
8 314	4 633	1 00	0 00	BrD ATOM	1357	HH21	ARG	80	-4 590
8 647	5 326	1 00	0.00	BrD ATOM	1358	HH22	ARG	80	-4 293
7 983	3 754	1.00	0.00	BrD ATOM	1359	C	ARG	80	-3 305
3.568	2 114	1.00	0.00	BrD ATOM	1360	O	ARG	80	-4 417
3.922	2.502	1 00	0 00	BrD ATOM	1361	N	VAL	81	-3 116
2 536	1 293	1 00	0 00	BrD ATOM	1362	HN	VAL	81	-2 203
2.301	1.024	1.00	0 00	BrD ATOM	1363	CA	VAL	81	-4 231
1.738	0.799	1.00	0.00	BrD ATOM	1364	HA	VAL	81	-4 849
2 374	0 182	1 00	0 00	BrD ATOM	1365	CB	VAL	81	-3 742
0 556	-0.063	1.00	0 00	BrD ATOM	1366	HB	VAL	81	-3 104
0 068	0 546	1 00	0 00	BrD ATOM	1367	CG1	VAL	81	-2 926
1.057	-1.244	1.00	0.00	BrD ATOM	1368	HG11	VAL	81	-3 462
0.861	-2 159	1 00	0.00	BrD ATOM	1369	HG12	VAL	81	-1.973
0.545	-1 268	1 00	0.00	BrD ATOM	1370	HG13	VAL	81	-2 763
2.119	-1 146	1.00	0.00	BrD ATOM	1371	CG2	VAL	81	-4 916
0.287	-0.539	1.00	0.00	BrD ATOM	1372	HG21	VAL	81	-4 851
0.425	-1 608	1 00	0 00	BrD ATOM	1373	HG22	VAL	81	-5 841
0 215	-0 297	1 00	0.00	BrD ATOM	1374	HG23	VAL	81	-4 890
1 250	-0 050	1.00	0 00	BrD ATOM	1375	C	VAL	81	-5.069
1.206	1 957	1.00	0.00	BrD ATOM	1376	O	VAL	81	-6 293
1.339	1.964	1.00	0 00	BrD ATOM	1377	N	PHE	82	-4.400
0.610	2 937	1 00	0.00	BrD ATOM	1378	HN	PHE	82	-3 424
0.540	2 876	1 00	0 00	BrD ATOM	1379	CA	PHE	82	-5 079
0 070	4.108	1 00	0 00	BrD ATOM	1380	HA	PHE	82	-5 919

0.514	3.764	1.00	0.00	BrD ATOM	1381	CB	PHE	82	-4.131
0.833	4.899	1.00	0.00	BrD ATOM	1382	HB1	PHE	82	-3.486
0.220	5.511	1.00	0.00	BrD ATOM	1383	HB2	PHE	82	-4.712
1.484	5.536	1.00	0.00	BrD ATOM	1384	CG	PHE	82	-3.261
1.695	4.028	1.00	0.00	BrD ATOM	1385	CD1	PHE	82	-1.979
2.035	4.428	1.00	0.00	BrD ATOM	1386	HD1	PHE	82	-1.606
1.677	5.376	1.00	0.00	BrD ATOM	1387	CD2	PHE	82	-3.725
2.162	2.809	1.00	0.00	BrD ATOM	1388	HD2	PHE	82	-4.723
1.901	2.487	1.00	0.00	BrD ATOM	1389	CE1	PHE	82	-1.177
2.827	3.628	1.00	0.00	BrD ATOM	1390	HE1	PHE	82	-0.179
3.086	3.951	1.00	0.00	BrD ATOM	1391	CE2	PHE	82	-2.928
2.952	2.004	1.00	0.00	BrD ATOM	1392	HE2	PHE	82	-3.302
3.311	1.057	1.00	0.00	BrD ATOM	1393	CZ	PHE	82	-1.651
3.284	2.413	1.00	0.00	BrD ATOM	1394	HZ	PHE	82	-1.029
3.906	1.789	1.00	0.00	BrD ATOM	1395	C	PHE	82	-5.594
1.197	4.994	1.00	0.00	BrD ATOM	1396	O	PHE	82	-6.745
1.180	5.431	1.00	0.00	BrD ATOM	1397	N	THR	83	-4.740
2.185	5.241	1.00	0.00	BrD ATOM	1398	HN	THR	83	-3.841
2.149	4.852	1.00	0.00	BrD ATOM	1399	CA	THR	83	-5.119
3.337	6.048	1.00	0.00	BrD ATOM	1400	HA	THR	83	-5.427
2.977	7.019	1.00	0.00	BrD ATOM	1401	CB	THR	83	-3.927
4.282	6.216	1.00	0.00	BrD ATOM	1402	HB	THR	83	-3.525
4.516	5.240	1.00	0.00	BrD ATOM	1403	OG1	THR	83	-2.905
3.666	6.982	1.00	0.00	BrD ATOM	1404	HG1	THR	83	-3.138
3.699	7.913	1.00	0.00	BrD ATOM	1405	CG2	THR	83	-4.283
5.589	6.892	1.00	0.00	BrD ATOM	1406	HG21	THR	83	-4.813
6.222	6.196	1.00	0.00	BrD ATOM	1407	HG22	THR	83	-3.379
6.085	7.214	1.00	0.00	BrD ATOM	1408	HG23	THR	83	-4.910
5.391	7.749	1.00	0.00	BrD ATOM	1409	C	THR	83	-6.286
4.077	5.402	1.00	0.00	BrD ATOM	1410	O	THR	83	-7.073
4.735	6.082	1.00	0.00	BrD ATOM	1411	N	ASN	84	-6.391
3.956	4.082	1.00	0.00	BrD ATOM	1412	HN	ASN	84	-5.732
3.418	3.597	1.00	0.00	BrD ATOM	1413	CA	ASN	84	-7.458
4.609	3.334	1.00	0.00	BrD ATOM	1414	HA	ASN	84	-7.546
5.622	3.698	1.00	0.00	BrD ATOM	1415	CB	ASN	84	-7.113
4.640	1.844	1.00	0.00	BrD ATOM	1416	HB1	ASN	84	-7.095
3.629	1.464	1.00	0.00	BrD ATOM	1417	HB2	ASN	84	-6.138
5.086	1.716	1.00	0.00	BrD ATOM	1418	CG	ASN	84	-8.115
5.438	1.035	1.00	0.00	BrD ATOM	1419	OD1	ASN	84	-9.269
5.596	1.433	1.00	0.00	BrD ATOM	1420	ND2	ASN	84	-7.677
5.945	-0.111	1.00	0.00	BrD ATOM	1421	HD21	ASN	84	-6.745
5.778	-0.365	1.00	0.00	BrD ATOM	1422	HD22	ASN	84	-8.302
6.465	-0.655	1.00	0.00	BrD ATOM	1423	C	ASN	84	-8.788
3.893	3.544	1.00	0.00	BrD ATOM	1424	O	ASN	84	-9.745
4.477	4.051	1.00	0.00	BrD ATOM	1425	N	CYS	85	-8.842
2.623	3.150	1.00	0.00	BrD ATOM	1426	HN	CYS	85	-8.046
2.213	2.751	1.00	0.00	BrD ATOM	1427	CA	CYS	85	-10.058
1.827	3.291	1.00	0.00	BrD ATOM	1428	HA	CYS	85	-10.778
2.193	2.575	1.00	0.00	BrD ATOM	1429	CB	CYS	85	-9.765
0.354	2.995	1.00	0.00	BrD ATOM	1430	HB1	CYS	85	-8.806
0.277	2.504	1.00	0.00	BrD ATOM	1431	HB2	CYS	85	-9.732
0.193	3.926	1.00	0.00	BrD ATOM	1432	SG	CYS	85	-10.992
0.444	1.933	1.00	0.00	BrD ATOM	1433	HG	CYS	85	-10.844
0.144	1.033	1.00	0.00	BrD ATOM	1434	C	CYS	85	-10.645
1.965	4.692	1.00	0.00	BrD ATOM	1435	O	CYS	85	-11.842
2.203	4.854	1.00	0.00	BrD ATOM	1436	N	LYS	86	-9.794
1.817	5.701	1.00	0.00	BrD ATOM	1437	HN	LYS	86	-8.852
1.626	5.508	1.00	0.00	BrD ATOM	1438	CA	LYS	86	-10.228
1.921	7.089	1.00	0.00	BrD ATOM	1439	HA	LYS	86	-11.111
1.310	7.203	1.00	0.00	BrD ATOM	1440	CB	LYS	86	-9.137
1.395	8.023	1.00	0.00	BrD ATOM	1441	HB1	LYS	86	-9.063
0.325	7.903	1.00	0.00	BrD ATOM	1442	HB2	LYS	86	-9.416
1.616	9.043	1.00	0.00	BrD ATOM	1443	CG	LYS	86	-7.768
1.998	7.763	1.00	0.00	BrD ATOM	1444	HG1	LYS	86	-7.809
2.583	6.857	1.00	0.00	BrD ATOM	1445	HG2	LYS	86	-7.050
1.199	7.645	1.00	0.00	BrD ATOM	1446	CD	LYS	86	-7.325
2.892	8.910	1.00	0.00	BrD ATOM	1447	HD1	LYS	86	-6.477
3.478	8.590	1.00	0.00	BrD ATOM	1448	HD2	LYS	86	-8.140
3.548	9.177	1.00	0.00	BrD ATOM	1449	CE	LYS	86	-6.929
2.076	10.130	1.00	0.00	BrD ATOM	1450	HE1	LYS	86	-7.418
1.114	10.078	1.00	0.00	BrD ATOM	1451	HE2	LYS	86	-5.858
1.935	10.120	1.00	0.00	BrD ATOM	1452	NZ	LYS	86	-7.317
2.749	11.400	1.00	0.00	BrD ATOM	1453	HZ1	LYS	86	-8.019
2.174	11.909	1.00	0.00	BrD ATOM	1454	HZ2	LYS	86	-7.729
3.682	11.199	1.00	0.00	BrD ATOM	1455	HZ3	LYS	86	-6.482
2.874	12.008	1.00	0.00	BrD ATOM	1456	C	LYS	86	-10.579
3.360	7.456	1.00	0.00	BrD ATOM	1457	O	LYS	86	-11.293
3.603	8.429	1.00	0.00	BrD ATOM	1458	N	GLU	87	-10.076
4.314	6.676	1.00	0.00	BrD ATOM	1459	HN	GLU	87	-9.514
4.064	5.914	1.00	0.00	BrD ATOM	1460	CA	GLU	87	-10.350
5.724	6.926	1.00	0.00	BrD ATOM	1461	HA	GLU	87	-10.510
5.848	7.986	1.00	0.00	BrD ATOM	1462	CB	GLU	87	-9.158
6.583	6.498	1.00	0.00	BrD ATOM	1463	HB1	GLU	87	-9.513
7.572	6.249	1.00	0.00	BrD ATOM	1464	HB2	GLU	87	-8.706
6.141	5.622	1.00	0.00	BrD ATOM	1465	CG	GLU	87	-8.088
6.716	7.570	1.00	0.00	BrD ATOM	1466	HG1	GLU	87	-7.954
5.757	8.048	1.00	0.00	BrD ATOM	1467	HG2	GLU	87	-7.163
7.016	7.101	1.00	0.00	BrD ATOM	1468	CD	GLU	87	-8.446
7.740	8.629	1.00	0.00	BrD ATOM	1469	OE1	GLU	87	-9.092
8.751	8.283	1.00	0.00	BrD ATOM	1470	OE2	GLU	87	-8.079
7.531	9.805	1.00	0.00	BrD ATOM	1471	C	GLU	87	-11.604
6.172	6.183	1.00	0.00	BrD ATOM	1472	O	GLU	87	-12.542
6.692	6.787	1.00	0.00	BrD ATOM	1473	N	TYR	88	-11.617
5.962	4.871	1.00	0.00	BrD ATOM	1474	HN	TYR	88	-10.840
5.541	4.446	1.00	0.00	BrD ATOM	1475	CA	TYR	88	-12.759
6.339	4.046	1.00	0.00	BrD ATOM	1476	HA	TYR	88	-13.070
7.330	4.344	1.00	0.00	BrD ATOM	1477	CB	TYR	88	-12.361
6.363	2.568	1.00	0.00	BrD ATOM	1478	HB1	TYR	88	-11.310
6.602	2.489	1.00	0.00	BrD ATOM	1479	HB2	TYR	88	-12.537
5.388	2.139	1.00	0.00	BrD ATOM	1480	CG	TYR	88	-13.128
7.376	1.748	1.00	0.00	BrD ATOM	1481	CD1	TYR	88	-12.606
8.640	1.505	1.00	0.00	BrD ATOM	1482	HD1	TYR	88	-11.639
8.896	1.914	1.00	0.00	BrD ATOM	1483	CD2	TYR	88	-14.372
7.066	1.213	1.00	0.00	BrD ATOM	1484	HD2	TYR	88	-14.792
6.087	1.392	1.00	0.00	BrD ATOM	1485	CE1	TYR	88	-13.302
9.568	0.755	1.00	0.00	BrD ATOM	1486	HE1	TYR	88	-12.880
10.546	0.578	1.00	0.00	BrD ATOM	1487	CE2	TYR	88	-15.075
7.989	0.462	1.00	0.00	BrD ATOM	1488	HE2	TYR	88	-16.042
7.730	0.055	1.00	0.00	BrD ATOM	1489	CZ	TYR	88	-14.536
9.238	0.236	1.00	0.00	BrD ATOM	1490	OH	TYR	88	-15.233
10.159	-0.512	1.00	0.00	BrD ATOM	1491	HH	TYR	88	-15.995
10.465	-0.014	1.00	0.00	BrD ATOM	1492	C	TYR	88	-13.923
5.374	4.256	1.00	0.00	BrD ATOM	1493	O	TYR	88	-14.369
4.711	3.320	1.00	0.00	BrD ATOM	1494	N	ASN	89	-14.408
5.298	5.492	1.00	0.00	BrD ATOM	1495	HN	ASN	89	-14.012
5.852	6.195	1.00	0.00	BrD ATOM	1496	CA	ASN	89	-15.518
4.414	5.827	1.00	0.00	BrD ATOM	1497	HA	ASN	89	-16.155
4.336	4.958	1.00	0.00	BrD ATOM	1498	CB	ASN	89	-14.996
3.023	6.192	1.00	0.00	BrD ATOM	1499	HB1	ASN	89	-15.816
2.421	6.557	1.00	0.00	BrD ATOM	1500	HB2	ASN	89	-14.578
2.559	5.311	1.00	0.00	BrD ATOM	1501	CG	ASN	89	-13.925
3.072	7.263	1.00	0.00	BrD ATOM	1502	OD1	ASN	89	-13.552
4.147	7.734	1.00	0.00	BrD ATOM	1503	ND2	ASN	89	-13.424
1.906	7.655	1.00	0.00	BrD ATOM	1504	HD21	ASN	89	-13.770
1.090	7.236	1.00	0.00	BrD ATOM	1505	HD22	ASN	89	-12.731
1.909	8.347	1.00	0.00	BrD ATOM	1506	C	ASN	89	-16.332
4.982	6.985	1.00	0.00	BrD ATOM	1507	O	ASN	89	-16.088
4.658	8.147	1.00	0.00	BrD ATOM	1508	N	ALA	90	-17.296
5.836	6.659	1.00	0.00	BrD ATOM	1509	HN	ALA	90	-17.438
6.058	5.715	1.00	0.00	BrD ATOM	1510	CA	ALA	90	-18.142
6.458	7.670	1.00	0.00	BrD ATOM	1511	HA	ALA	90	-17.525
7.122	8.258	1.00	0.00	BrD ATOM	1512	CB	ALA	90	-19.228
7.291	7.006	1.00	0.00	BrD ATOM	1513	HB1	ALA	90	-19.280
7.045	5.956	1.00	0.00	BrD ATOM	1514	HB2	ALA	90	-18.997
8.340	7.119	1.00	0.00	BrD ATOM	1515	HB3	ALA	90	-20.179
7.081	7.473	1.00	0.00	BrD ATOM	1516	C	ALA	90	-18.764
5.414	8.594	1.00	0.00	BrD ATOM	1517	O	ALA	90	-18.728
5.557	9.817	1.00	0.00	BrD ATOM	1518	N	PRO	91	-19.346
4.347	8.021	1.00	0.00	BrD ATOM	1519	CA	PRO	91	-20.000
3.290	8.783	1.00	0.00	BrD ATOM	1520	HA	PRO	91	-20.495
3.681	9.659	1.00	0.00	BrD ATOM	1521	CB	PRO	91	-21.048
2.740	7.800	1.00	0.00	BrD ATOM	1522	HB1	PRO	91	-20.932
1.670	7.715	1.00	0.00	BrD ATOM	1523	HB2	PRO	91	-22.038
2.966	8.169	1.00	0.00	BrD ATOM	1524	CG	PRO	91	-20.794
3.419	6.483	1.00	0.00	BrD ATOM	1525	HG1	PRO	91	-20.778
2.684	5.692	1.00	0.00	BrD ATOM	1526	HG2	PRO	91	-21.566
4.151	6.296	1.00	0.00	BrD ATOM	1527	CD	PRO	91	-19.456
4.095	6.587	1.00	0.00	BrD ATOM	1528	HD1	PRO	91	-18.670
3.436	6.247	1.00	0.00	BrD ATOM	1529	HD2	PRO	91	-19.450
5.018	6.027	1.00	0.00	BrD ATOM	1530	C	PRO	91	-19.035
2.183	9.196	1.00	0.00	BrD ATOM	1531	O	PRO	91	-19.458
1.079	9.540	1.00	0.00	BrD ATOM	1532	N	GLU	92	-17.736
2.481	9.160	1.00	0.00	BrD ATOM	1533	HN	GLU	92	-17.462
3.377	8.873	1.00	0.00	BrD ATOM	1534	CA	GLU	92	-16.703
1.506	9.521	1.00	0.00	BrD ATOM	1535	HA	GLU	92	-15.779
1.838	9.083	1.00	0.00	BrD ATOM	1536	CB	GLU	92	-16.529
1.439	11.039	1.00	0.00	BrD ATOM	1537	HB1	GLU	92	-15.786
0.690	11.272	1.00	0.00	BrD ATOM	1538	HB2	GLU	92	-16.182
2.399	11.393	1.00	0.00	BrD ATOM	1539	CG	GLU	92	-17.805
1.092	11.778	1.00	0.00	BrD ATOM	1540	HG1	GLU	92	-18.550
1.831	11.537	1.00	0.00	BrD ATOM	1541	HG2	GLU	92	-18.143
0.119	11.452	1.00	0.00	BrD ATOM	1542	CD	GLU	92	-17.622
1.062	13.283	1.00	0.00	BrD ATOM	1543	OE1	GLU	92	-18.536
1.517	14.001	1.00	0.00	BrD ATOM	1544	OE2	GLU	92	-16.564
0.581	13.743	1.00	0.00	BrD ATOM	1545	C	GLU	92	-17.029
0.119	8.974	1.00	0.00	BrD ATOM	1546	O	GLU	92	-16.862
0.887	9.663	1.00	0.00	BrD ATOM	1547	N	SER	93	-17.508
0.081	7.736	1.00	0.00	BrD ATOM	1548	HN	SER	93	-17.620
0.919	7.240	1.00	0.00	BrD ATOM	1549	CA	SER	93	-17.863
1.176	7.092	1.00	0.00	BrD ATOM	1550	HA	SER	93	-18.677
1.616	7.649	1.00	0.00	BrD ATOM	1551	CB	SER	93	-18.317
0.925	5.653	1.00	0.00	BrD ATOM	1552	HB1	SER	93	-17.475
1.052	4.986	1.00	0.00	BrD ATOM	1553	HB2	SER	93	-18.695
0.084	5.568	1.00	0.00	BrD ATOM	1554	OG	SER	93	-19.339
1.830	5.274	1.00	0.00	BrD ATOM	1555	HG	SER	93	-19.610
1.648	4.371	1.00	0.00	BrD ATOM	1556	C	SER	93	-16.686
2.141	7.099	1.00	0.00	BrD ATOM	1557	O	SER	93	-15.700
1.932	7.807	1.00	0.00	BrD ATOM	1558	N	GLU	94	-16.790
3.194	6.298	1.00	0.00	BrD ATOM	1559	HN	GLU	94	-17.598
3.303	5.754	1.00	0.00	BrD ATOM	1560	CA	GLU	94	-15.729
4.186	6.204	1.00	0.00	BrD ATOM	1561	HA	GLU	94	-15.574
4.596	7.191	1.00	0.00	BrD ATOM	1562	CB	GLU	94	-16.144
5.314	5.258	1.00	0.00	BrD ATOM	1563	HB1	GLU	94	-16.411
4.887	4.302	1.00	0.00	BrD ATOM	1564	HB2	GLU	94	-17.006
5.817	5.671	1.00	0.00	BrD ATOM	1565	CG	GLU	94	-15.054
6.346	5.031	1.00	0.00	BrD ATOM	1566	HG1	GLU	94	-14.187
5.849	4.622	1.00	0.00	BrD ATOM	1567	HG2	GLU	94	-14.797
6.793	5.981	1.00	0.00	BrD ATOM	1568	CD	GLU	94	-15.479
7.446	4.078	1.00	0.00	BrD ATOM	1569	OE1	GLU	94	-16.617
7.382	3.568	1.00	0.00	BrD ATOM	1570	OE2	GLU	94	-14.673
8.370	3.840	1.00	0.00	BrD ATOM	1571	C	GLU	94	-14.422
3.556	5.725	1.00	0.00	BrD ATOM	1572	O	GLU	94	-13.351
4.143	5.876	1.00	0.00	BrD ATOM	1573	N	TYR	95	-14.510
2.357	5.150	1.00	0.00	BrD ATOM	1574	HN	TYR	95	-15.387
1.930	5.057	1.00	0.00	BrD ATOM	1575	CA	TYR	95	-13.327
1.658	4.663	1.00	0.00	BrD ATOM	1576	HA	TYR	95	-12.919
2.227	3.841	1.00	0.00	BrD ATOM	1577	CB	TYR	95	-13.704
0.260	4.166	1.00	0.00	BrD ATOM	1578	HB1	TYR	95	-14.448
0.160	4.827	1.00	0.00	BrD ATOM	1579	HB2	TYR	95	-12.825
0.367	4.176	1.00	0.00	BrD ATOM	1580	CG	TYR	95	-14.270
0.244	2.762	1.00	0.00	BrD ATOM	1581	CD1	TYR	95	-14.933
1.350	2.245	1.00	0.00	BrD ATOM	1582	HD1	TYR	95	-15.041
2.232	2.859	1.00	0.00	BrD ATOM	1583	CD2	TYR	95	-14.141
0.880	1.956	1.00	0.00	BrD ATOM	1584	HD2	TYR	95	-13.630
1.749	2.343	1.00	0.00	BrD ATOM	1585	CE1	TYR	95	-15.450
1.337	0.963	1.00	0.00	BrD ATOM	1586	HE1	TYR	95	-15.961
2.208	0.579	1.00	0.00	BrD ATOM	1587	CE2	TYR	95	-14.656
0.901	0.673	1.00	0.00	BrD ATOM	1588	HE2	TYR	95	-14.546
1.785	0.062	1.00	0.00	BrD ATOM	1589	CZ	TYR	95	-15.310
0.210	0.182	1.00	0.00	BrD ATOM	1590	OH	TYR	95	-15.823
0.193	-1.095	1.00	0.00	BrD ATOM	1591	HH	TYR	95	-16.730
0.508	-1.079	1.00	0.00	BrD ATOM	1592	C	TYR	95	-12.274
1.552	5.761	1.00	0.00	BrD ATOM	1593	O	TYR	95	-11.076
1.511	5.485	1.00	0.00	BrD ATOM	1594	N	TYR	96	-12.733
1.513	7.007	1.00	0.00	BrD ATOM	1595	HN	TYR	96	-13.700
1.553	7.161	1.00	0.00	BrD ATOM	1596	CA	TYR	96	-11.835
1.421	8.152	1.00	0.00	BrD ATOM	1597	HA	TYR	96	-11.033
0.746	7.889	1.00	0.00	BrD ATOM	1598	CB	TYR	96	-12.581
0.860	9.365	1.00	0.00	BrD ATOM	1599	HB1	TYR	96	-13.397
1.522	9.615	1.00	0.00	BrD ATOM	1600	HB2	TYR	96	-12.977
0.114	9.116	1.00	0.00	BrD ATOM	1601	CG	TYR	96	-11.712
0.708	10.594	1.00	0.00	BrD ATOM	1602	CD1	TYR	96	-10.351
0.458	10.477	1.00	0.00	BrD ATOM	1603	HD1	TYR	96	-9.918
0.275	9.493	1.00	0.00	BrD ATOM	1604	CD2	TYR	96	-12.252
0.815	11.870	1.00	0.00	BrD ATOM	1605	HD2	TYR	96	-13.308
1.009	11.979	1.00	0.00	BrD ATOM	1606	CE1	TYR	96	-9.551
0.319	11.594	1.00	0.00	BrD ATOM	1607	HE1	TYR	96	-8.495
0.125	11.480	1.00	0.00	BrD ATOM	1608	CE2	TYR	96	-11.458
0.677	12.993	1.00	0.00	BrD ATOM	1609	HE2	TYR	96	-11.895
0.763	13.977	1.00	0.00	BrD ATOM	1610	CZ	TYR	96	-10.109
0.429	12.849	1.00	0.00	BrD ATOM	1611	OH	TYR	96	-9.315
0.291	13.964	1.00	0.00	BrD ATOM	1612	HH	TYR	96	-8.479
0.742	13.821	1.00	0.00	BrD ATOM	1613	C	TYR	96	-11.238
2.783	8.497	1.00	0.00	BrD ATOM	1614	O	TYR	96	-10.238
2.868	9.211	1.00	0.00	BrD ATOM	1615	N	LYS	97	-11.857
3.849	7.995	1.00	0.00	BrD ATOM	1616	HN	LYS	97	-12.650
3.728	7.435	1.00	0.00	BrD ATOM	1617	CA	LYS	97	-11.390
5.200	8.256	1.00	0.00	BrD ATOM	1618	HA	LYS	97	-11.067
5.248	9.285	1.00	0.00	BrD ATOM	1619	CB	LYS	97	-12.547
6.183	8.044	1.00	0.00	BrD ATOM	1620	HB1	LYS	97	-13.075
5.901	7.145	1.00	0.00	BrD ATOM	1621	HB2	LYS	97	-13.223
6.110	8.884	1.00	0.00	BrD ATOM	1622	CG	LYS	97	-12.120
7.632	7.902	1.00	0.00	BrD ATOM	1623	HG1	LYS	97	-11.914
7.826	6.862	1.00	0.00	BrD ATOM	1624	HG2	LYS	97	-11.227
7.795	8.487	1.00	0.00	BrD ATOM	1625	CD	LYS	97	-13.205
8.584	8.379	1.00	0.00	BrD ATOM	1626	HD1	LYS	97	-14.156
8.255	7.989	1.00	0.00	BrD ATOM	1627	HD2	LYS	97	-12.986
9.576	8.013	1.00	0.00	BrD ATOM	1628	CE	LYS	97	-13.282
8.625	9.897	1.00	0.00	BrD ATOM	1629	HE1	LYS	97	-13.091
7.633	10.281	1.00	0.00	BrD ATOM	1630	HE2	LYS	97	-12.527
9.304	10.265	1.00	0.00	BrD ATOM	1631	NZ	LYS	97	-14.617
9.080	10.374	1.00	0.00	BrD ATOM	1632	HZ1	LYS	97	-14.760
10.082	10.135	1.00	0.00	BrD ATOM	1633	HZ2	LYS	97	-15.368
8.517	9.926	1.00	0.00	BrD ATOM	1634	HZ3	LYS	97	-14.685
8.968	11.406	1.00	0.00	BrD ATOM	1635	C	LYS	97	-10.212
5.550	7.349	1.00	0.00	BrD ATOM	1636	O	LYS	97	-9.123
5.870	7.824	1.00	0.00	BrD ATOM	1637	N	CYS	98	-10.443
5.490	6.040	1.00	0.00	BrD ATOM	1638	HN	CYS	98	-11.334
5.233	5.724	1.00	0.00	BrD ATOM	1639	CA	CYS	98	-9.408
5.811	5.062	1.00	0.00	BrD ATOM	1640	HA	CYS	98	-9.253
6.879	5.086	1.00	0.00	BrD ATOM	1641	CB	CYS	98	-9.862
5.408	3.660	1.00	0.00	BrD ATOM	1642	HB1	CYS	98	-9.000
5.351	3.012	1.00	0.00	BrD ATOM	1643	HB2	CYS	98	-10.337
4.440	3.707	1.00	0.00	BrD ATOM	1644	SG	CYS	98	-11.036
6.562	2.916	1.00	0.00	BrD ATOM	1645	HG	CYS	98	-11.755
6.695	3.538	1.00	0.00	BrD ATOM	1646	C	CYS	98	-8.093
5.121	5.405	1.00	0.00	BrD ATOM	1647	O	CYS	98	-7.040
5.757	5.442	1.00	0.00	BrD ATOM	1648	N	ALA	99	-8.159
3.820	5.668	1.00	0.00	BrD ATOM	1649	HN	ALA	99	-9.028
3.368	5.644	1.00	0.00	BrD ATOM	1650	CA	ALA	99	-6.975
3.066	6.046	1.00	0.00	BrD ATOM	1651	HA	ALA	99	-6.290
3.066	5.214	1.00	0.00	BrD ATOM	1652	CB	ALA	99	-7.339
1.623	6.363	1.00	0.00	BrD ATOM	1653	HB1	ALA	99	-8.281
1.597	6.890	1.00	0.00	BrD ATOM	1654	HB2	ALA	99	-7.425
1.063	5.443	1.00	0.00	BrD ATOM	1655	HB3	ALA	99	-6.568
1.185	6.980	1.00	0.00	BrD ATOM	1656	C	ALA	99	-6.293
3.721	7.232	1.00	0.00	BrD ATOM	1657	O	ALA	99	-5.091
3.963	7.207	1.00	0.00	BrD ATOM	1658	N	ASN	100	-7.080
4.054	8.247	1.00	0.00	BrD ATOM	1659	HN	ASN	100	-8.039
3.848	8.199	1.00	0.00	BrD ATOM	1660	CA	ASN	100	-6.550
4.702	9.438	1.00	0.00	BrD ATOM	1661	HA	ASN	100	-5.922
3.988	9.949	1.00	0.00	BrD ATOM	1662	CB	ASN	100	-7.697

5.116	10.363	1.00	0.00	BrD ATOM	1663	HB1	ASN	100	-8.587	-
4.570	10.089	1.00	0.00	BrD ATOM	1664	HB2	ASN	100	-7 879	-
6 174	10.247	1.00	0 00	BrD ATOM	1665	CG	ASN	100	-7.395	-
4.838	11 822	1 00	0.00	BrD ATOM	1666	OD1	ASN	100	-7 283	-
3 684	12 236	1 00	0 00	BrD ATOM	1667	ND2	ASN	100	-7 266	-
5 898	12.611	1 00	0 00	BrD ATOM	1668	HD21	ASN	100	-7 370	-
6.787	12 212	1 00	0 00	BrD ATOM	1669	HD22	ASN	100	-7 072	-
5 748	13 560	1 00	0 00	BrD ATOM	1670	C	ASN	100	-5 711	-
5.922	9 069	1.00	0 00	BrD ATOM	1671	O	ASN	100	-4 740	-
6 251	9 753	1 00	0.00	BrD ATOM	1672	N	ILE	101	-6.088	-
6 587	7.981	1 00	0.00	BrD ATOM	1673	HN	ILE	101	-6 870	-
6 277	7.481	1 00	0 00	BrD ATOM	1674	CA	ILE	101	-5 377	-
7 777	7 524	1 00	0 00	BrD ATOM	1675	HA	ILE	101	-5.132	-
8.370	8 394	1 00	0 00	BrD ATOM	1676	CB	ILE	101	-6.254	-
8.636	6 594	1 00	0 00	BrD ATOM	1677	HB	ILE	101	-6.469	-
8.061	5 705	1 00	0 00	BrD ATOM	1678	CG1	ILE	101	-7 569	-
8.996	7 290	1 00	0 00	BrD ATOM	1679	HG11	ILE	101	-8 112	-
8.090	7 513	1 00	0.00	BrD ATOM	1680	HG12	ILE	101	-7 350	-
9 516	8 212	1 00	0 00	BrD ATOM	1681	CG2	ILE	101	-5 509	-
9.894	6 177	1 00	0 00	BrD ATOM	1682	HG21	ILE	101	-6 221	-
10 659	5 902	1 00	0 00	BrD ATOM	1683	HG22	ILE	101	-4 905	-
10 244	7.001	1 00	0 00	BrD ATOM	1684	HG23	ILE	101	-4 874	-
9 673	5 333	1 00	0 00	BrD ATOM	1685	CD1	ILE	101	-8.470	-
9.885	6 461	1 00	0 00	BrD ATOM	1686	HD11	ILE	101	-9.158	-
10 406	7.109	1 00	0 00	BrD ATOM	1687	HD12	ILE	101	-7.869	-
10 604	5 922	1 00	0 00	BrD ATOM	1688	HD13	ILE	101	-9.024	-
9 281	5 758	1 00	0 00	BrD ATOM	1689	C	ILE	101	-4 084	-
7 408	6 802	1 00	0 00	BrD ATOM	1690	O	ILE	101	-2 993	-
7.580	7 345	1 00	0 00	BrD ATOM	1691	N	LEU	102	-4.206	-
6 890	5 579	1.00	0 00	BrD ATOM	1692	HN	LEU	102	-5 100	-
6 770	5 196	1 00	0 00	BrD ATOM	1693	CA	LEU	102	-3 033	-
6 488	4 800	1 00	0 00	BrD ATOM	1694	HA	LEU	102	-2 519	-
7 384	4 485	1 00	0 00	BrD ATOM	1695	CB	LEU	102	-3 454	-
5.690	3 565	1.00	0.00	BrD ATOM	1696	HB1	LEU	102	-4.530	-
5.734	3.485	1 00	0 00	BrD ATOM	1697	HB2	LEU	102	-3.164	-
4 661	3 717	1.00	0 00	BrD ATOM	1698	CG	LEU	102	-2 852	-
6 166	2 236	1.00	0 00	BrD ATOM	1699	HG	LEU	102	-2 990	-
5 394	1 493	1 00	0.00	BrD ATOM	1700	CD1	LEU	102	-3 570	-
7.417	1 745	1 00	0 00	BrD ATOM	1701	HD11	LEU	102	-4 201	-
7 803	2 533	1 00	0 00	BrD ATOM	1702	HD12	LEU	102	-2 843	-
8.165	1 468	1 00	0 00	BrD ATOM	1703	HD13	LEU	102	-4 180	-
7 170	0 887	1 00	0 00	BrD ATOM	1704	CD2	LEU	102	-1 353	-
6.418	2 376	1 00	0 00	BrD ATOM	1705	HD21	LEU	102	-1 167	-
7 481	2.412	1 00	0.00	BrD ATOM	1706	HD22	LEU	102	-0 992	-
5 959	3.285	1 00	0 00	BrD ATOM	1707	HD23	LEU	102	-0.833	-
5 992	1 529	1.00	0.00	BrD ATOM	1708	C	LEU	102	-2 087	-
5.649	5 649	1 00	0 00	BrD ATOM	1709	O	LEU	102	-0 868	-
5 770	5 546	1 00	0 00	BrD ATOM	1710	N	GLU	103	-2 661	-
4 792	6 486	1 00	0 00	BrD ATOM	1711	HN	GLU	103	-3 639	-
4 747	6 528	1 00	0 00	BrD ATOM	1712	CA	GLU	103	-1 872	-
3 948	7 369	1 00	0.00	BrD ATOM	1713	HA	GLU	103	-1.199	-
3.364	6 758	1.00	0.00	BrD ATOM	1714	CB	GLU	103	-2 781	-
3.002	8 159	1.00	0 00	BrD ATOM	1715	HB1	GLU	103	-3.230	-
2 297	7 475	1 00	0 00	BrD ATOM	1716	HB2	GLU	103	-3.559	-
3.579	8 627	1 00	0 00	BrD ATOM	1717	CG	GLU	103	-2.060	-
2 222	9 242	1 00	0.00	BrD ATOM	1718	HG1	GLU	103	-2 356	-
2 611	10 205	1 00	0 00	BrD ATOM	1719	HG2	GLU	103	-0 999	-
2.356	9 112	1.00	0.00	BrD ATOM	1720	CD	GLU	103	-2 373	-
0.740	9.200	1.00	0 00	BrD ATOM	1721	OE1	GLU	103	-2 248	-
0.077	10.251	1.00	0.00	BrD ATOM	1722	OE2	GLU	103	-2 745	-
0 242	8 117	1.00	0 00	BrD ATOM	1723	C	GLU	103	-1 052	-
4 808	8 322	1 00	0 00	BrD ATOM	1724	O	GLU	103	0 175	-
4.759	8 317	1 00	0 00	BrD ATOM	1725	N	LYS	104	-1.740	-
5 627	9.114	1.00	0 00	BrD ATOM	1726	HN	LYS	104	-2 720	-
5 629	9 066	1.00	0 00	BrD ATOM	1727	CA	LYS	104	-1 072	-
6 511	10.062	1 00	0 00	BrD ATOM	1728	HA	LYS	104	-0 569	-
5 894	10 792	1.00	0 00	BrD ATOM	1729	CB	LYS	104	-2.097	-
7.395	10 777	1 00	0.00	BrD ATOM	1730	HB1	LYS	104	-2 976	-
7 479	10 157	1.00	0 00	BrD ATOM	1731	HB2	LYS	104	-1 670	-
8.377	10 917	1.00	0 00	BrD ATOM	1732	CG	LYS	104	-2 520	-
6.861	12 136	1.00	0 00	BrD ATOM	1733	HG1	LYS	104	-3 354	-
7 445	12 497	1 00	0 00	BrD ATOM	1734	HG2	LYS	104	-1 691	-
6.951	12 822	1 00	0 00	BrD ATOM	1735	CD	LYS	104	-2 938	-
5 401	12 056	1 00	0 00	BrD ATOM	1736	HD1	LYS	104	-2 817	-
5.059	11 039	1 00	0 00	BrD ATOM	1737	HD2	LYS	104	-2 306	-
4 819	12 712	1 00	0 00	BrD ATOM	1738	CE	LYS	104	-4 387	-
5 210	12 469	1 00	0 00	BrD ATOM	1739	HE1	LYS	104	-4 975	-
5.002	11.587	1 00	0.00	BrD ATOM	1740	HE2	LYS	104	-4.741	-
6.120	12 930	1.00	0 00	BrD ATOM	1741	NZ	LYS	104	-4 547	-
4.085	13 432	1 00	0.00	BrD ATOM	1742	HZ1	LYS	104	-5 135	-
4.384	14 236	1 00	0 00	BrD ATOM	1743	HZ2	LYS	104	-5.004	-
3 277	12 964	1 00	0 00	BrD ATOM	1744	HZ3	LYS	104	-3 618	-
3.785	13.788	1.00	0 00	BrD ATOM	1745	C	LYS	104	-0 039	-
7 383	9.357	1 00	0 00	BrD ATOM	1746	O	LYS	104	1 021	-
7 678	9 910	1 00	0 00	BrD ATOM	1747	N	PHE	105	-0.357	-
7.796	8.135	1 00	0 00	BrD ATOM	1748	HN	PHE	105	-1 217	-
7.528	7 749	1.00	0 00	BrD ATOM	1749	CA	PHE	105	0.541	-
8.636	7.352	1 00	0.00	BrD ATOM	1750	HA	PHE	105	0 954	-
9 385	8 011	1.00	0 00	BrD ATOM	1751	CB	PHE	105	-0 229	-
9 331	6.228	1 00	0 00	BrD ATOM	1752	HB1	PHE	105	0 455	-
9 569	5.426	1.00	0 00	BrD ATOM	1753	HB2	PHE	105	-0 992	-
8.662	5 857	1.00	0 00	BrD ATOM	1754	CG	PHE	105	-0.899	-
10.604	6 658	1 00	0.00	BrD ATOM	1755	CD1	PHE	105	-0 202	-
11 559	7.381	1.00	0 00	BrD ATOM	1756	HD1	PHE	105	0.833	-
11.381	7.633	1.00	0.00	BrD ATOM	1757	CD2	PHE	105	-2.226	-
10.844	6 342	1.00	0.00	BrD ATOM	1758	HD2	PHE	105	-2.779	-
10.106	5 780	1 00	0.00	BrD ATOM	1759	CE1	PHE	105	-0 816	-
12 730	7.780	1.00	0.00	BrD ATOM	1760	HE1	PHE	105	-0.262	-
13 467	8 342	1.00	0.00	BrD ATOM	1761	CE2	PHE	105	-2.846	-
12 013	6 738	1.00	0.00	BrD ATOM	1762	HE2	PHE	105	-3.881	-
12 188	6 485	1.00	0.00	BrD ATOM	1763	CZ	PHE	105	-2 140	-
12 958	7 458	1 00	0.00	BrD ATOM	1764	HZ	PHE	105	-2.623	-
13 873	7.768	1 00	0 00	BrD ATOM	1765	C	PHE	105	1 684	-
7 817	6 766	1 00	0 00	BrD ATOM	1766	O	PHE	105	2.845	-
7 998	7 133	1.00	0.00	BrD ATOM	1767	N	PHE	106	1 347	-
6 917	5 849	1 00	0.00	BrD ATOM	1768	HN	PHE	106	0 405	-
6.824	5 595	1 00	0.00	BrD ATOM	1769	CA	PHE	106	2.344	-
6.075	5 202	1 00	0 00	BrD ATOM	1770	HA	PHE	106	2 956	-
6.711	4.579	1 00	0 00	BrD ATOM	1771	CB	PHE	106	1 665	-
5.021	4 325	1 00	0 00	BrD ATOM	1772	HB1	PHE	106	0 985	-
5 512	3 644	1.00	0 00	BrD ATOM	1773	HB2	PHE	106	1 110	-
4 341	4 954	1.00	0 00	BrD ATOM	1774	CG	PHE	106	2 633	-
4 213	3 510	1 00	0.00	BrD ATOM	1775	CD1	PHE	106	3.519	-
4 836	2 649	1 00	0.00	BrD ATOM	1776	HD1	PHE	106	3.508	-
5 913	2 565	1 00	0 00	BrD ATOM	1777	CD2	PHE	106	2.662	-
2 831	3.612	1.00	0 00	BrD ATOM	1778	HD2	PHE	106	1 974	-
2 333	4.279	1.00	0 00	BrD ATOM	1779	CE1	PHE	106	4 413	-
4.098	1.898	1 00	0 00	BrD ATOM	1780	HE1	PHE	106	5.098	-
4 598	1.229	1 00	0 00	BrD ATOM	1781	CE2	PHE	106	3 548	-
2 086	2 857	1 00	0 00	BrD ATOM	1782	HE2	PHE	106	3.562	-
1 010	2 946	1.00	0 00	BrD ATOM	1783	CZ	PHE	106	4 432	-
2 721	2 005	1.00	0.00	BrD ATOM	1784	HZ	PHE	106	5 127	-
2 142	1 417	1 00	0 00	BrD ATOM	1785	C	PHE	106	3 236	-
5 388	6 230	1.00	0.00	BrD ATOM	1786	O	PHE	106	4 439	-
5 637	6.282	1 00	0.00	BrD ATOM	1787	N	PHE	107	2.643	-
4 516	7 043	1 00	0 00	BrD ATOM	1788	HN	PHE	107	1.679	-
4 349	6 948	1 00	0 00	BrD ATOM	1789	CA	PHE	107	3 401	-
3.784	8 058	1.00	0 00	BrD ATOM	1790	HA	PHE	107	4 035	-
3 076	7 543	1.00	0 00	BrD ATOM	1791	CB	PHE	107	2 462	-
3 014	8 995	1.00	0 00	BrD ATOM	1792	HB1	PHE	107	1 719	-
3 692	9 384	1 00	0 00	BrD ATOM	1793	HB2	PHE	107	3 040	-
2 618	9 817	1.00	0 00	BrD ATOM	1794	CG	PHE	107	1 741	-
1 858	8 345	1 00	0 00	BrD ATOM	1795	CD1	PHE	107	1 007	-
0 971	9 117	1.00	0 00	BrD ATOM	1796	HD1	PHE	107	0 954	-
1 118	10 186	1 00	0 00	BrD ATOM	1797	CD2	PHE	107	1.798	-
1 652	6 972	1 00	0 00	BrD ATOM	1798	HD2	PHE	107	2.368	-
2.334	6 357	1 00	0 00	BrD ATOM	1799	CE1	PHE	107	0 345	
0 095	8 537	1.00	0 00	BrD ATOM	1800	HE1	PHE	107	-0 224	
0 776	9.151	1.00	0 00	BrD ATOM	1801	CE2	PHE	107	1 137	-
0 588	6.387	1 00	0 00	BrD ATOM	1802	HE2	PHE	107	1 192	-
0 439	5 318	1 00	0.00	BrD ATOM	1803	CZ	PHE	107	0.410	
0 286	7.171	1 00	0 00	BrD ATOM	1804	HZ	PHE	107	-0 108	
1 118	6 718	1 00	0.00	BrD ATOM	1805	C	PHE	107	4.287	-
4 727	8.867	1 00	0.00	BrD ATOM	1806	O	PHE	107	5.369	-
4 345	9 312	1 00	0.00	BrD ATOM	1807	N	SER	108	3.825	-
5 960	9.054	1.00	0 00	BrD ATOM	1808	HN	SER	108	2 968	-
6 218	8 654	1 00	0.00	BrD ATOM	1809	CA	SER	108	4 607	-
6 959	9 773	1.00	0.00	BrD ATOM	1810	HA	SER	108	4 981	-
6 503	10 678	1 00	0 00	BrD ATOM	1811	CB	SER	108	3.740	-
8 166	10 136	1 00	0 00	BrD ATOM	1812	HB1	SER	108	2.987	-
7 864	10 848	1 00	0 00	BrD ATOM	1813	HB2	SER	108	3.262	-
8 546	9.245	1 00	0.00	BrD ATOM	1814	OG	SER	108	4 521	-
9 200	10.711	1.00	0 00	BrD ATOM	1815	HG	SER	108	4 902	-
9 739	10 014	1.00	0 00	BrD ATOM	1816	C	SER	108	5.784	-
7 395	8 915	1.00	0 00	BrD ATOM	1817	O	SER	108	6 887	-
7.618	9.413	1 00	0 00	BrD ATOM	1818	N	LYS	109	5 540	-
7 475	7 613	1 00	0.00	BrD ATOM	1819	HN	LYS	109	4.643	-
7 256	7.283	1.00	0 00	BrD ATOM	1820	CA	LYS	109	6 578	-
7 819	6.656	1.00	0 00	BrD ATOM	1821	HA	LYS	109	7 113	-
8 679	7.032	1 00	0 00	BrD ATOM	1822	CB	LYS	109	5 950	-
8.163	5 306	1 00	0 00	BrD ATOM	1823	HB1	LYS	109	4.898	-
7 922	5 340	1 00	0.00	BrD ATOM	1824	HB2	LYS	109	6.421	-
7 566	4.542	1 00	0 00	BrD ATOM	1825	CG	LYS	109	6 090	-
9 626	4.926	1 00	0.00	BrD ATOM	1826	HG1	LYS	109	5.522	-
9 811	4 026	1 00	0 00	BrD ATOM	1827	HG2	LYS	109	7.133	-
9.844	4 748	1.00	0.00	BrD ATOM	1828	CD	LYS	109	5.577	-
10 535	6 029	1 00	0.00	BrD ATOM	1829	HD1	LYS	109	6 413	-
10 864	6 629	1 00	0 00	BrD ATOM	1830	HD2	LYS	109	4 885	-
9 981	6.646	1.00	0 00	BrD ATOM	1831	CE	LYS	109	4 866	-
11 751	5 462	1.00	0 00	BrD ATOM	1832	HE1	LYS	109	5 179	-
11 889	4.438	1.00	0.00	BrD ATOM	1833	HE2	LYS	109	3.801	-
11.575	5 491	1 00	0 00	BrD ATOM	1834	NZ	LYS	109	5.175	-
12 986	6.235	1 00	0 00	BrD ATOM	1835	HZ1	LYS	109	6.202	-
13 148	6 254	1 00	0 00	BrD ATOM	1836	HZ2	LYS	109	4.715	-
13 808	5 795	1 00	0 00	BrD ATOM	1837	HZ3	LYS	109	4.831	-
12 892	7.212	1 00	0.00	BrD ATOM	1838	C	LYS	109	7.547	-
6 653	6.504	1.00	0 00	BrD ATOM	1839	O	LYS	109	8 761	-
6 842	6.428	1 00	0 00	BrD ATOM	1840	N	ILE	110	6 994	-
5 441	6 492	1.00	0 00	BrD ATOM	1841	HN	ILE	110	6.022	-
5 363	6.581	1 00	0 00	BrD ATOM	1842	CA	ILE	110	7.796	-
4 223	6 407	1.00	0.00	BrD ATOM	1843	HA	ILE	110	8.198	-
4 138	5.405	1 00	0.00	BrD ATOM	1844	CB	ILE	110	6 935	-
2 973	6 692	1.00	0 00	BrD ATOM	1845	HB	ILE	110	6 496	-
3.087	7.671	1.00	0 00	BrD ATOM	1846	CG1	ILE	110	5 811	-
2 844	5.654	1.00	0.00	BrD ATOM	1847	HG11	ILE	110	5.353	-
3.811	5 511	1.00	0.00	BrD ATOM	1848	HG12	ILE	110	5.068	-
2 153	6 026	1.00	0.00	BrD ATOM	1849	CG2	ILE	110	7.798	-
1 722	6 712	1 00	0.00	BrD ATOM	1850	HG21	ILE	110	8.756	-
1.945	6.264	1.00	0.00	BrD ATOM	1851	HG22	ILE	110	7.944	-
1.401	7.732	1.00	0.00	BrD ATOM	1852	HG23	ILE	110	7.311	-
0.938	6 152	1.00	0 00	BrD ATOM	1853	CD1	ILE	110	6 269	-
2.345	4 297	1.00	0 00	BrD ATOM	1854	HD11	ILE	110	6 222	-
3 153	3.583	1.00	0.00	BrD ATOM	1855	HD12	ILE	110	7.283	-
1 985	4.366	1 00	0.00	BrD ATOM	1856	HD13	ILE	110	5.623	-
1.540	3.971	1 00	0.00	BrD ATOM	1857	C	ILE	110	8.948	-
4.274	7 411	1.00	0 00	BrD ATOM	1858	O	ILE	110	10.104	-
4.045	7 060	1 00	0.00	BrD ATOM	1859	N	LYS	111	8.615	-
4.582	8 662	1.00	0.00	BrD ATOM	1860	HN	LYS	111	7 674	-
4.752	8 875	1.00	0 00	BrD ATOM	1861	CA	LYS	111	9 608	-
4 664	9 730	1 00	0 00	BrD ATOM	1862	HA	LYS	111	9 919	-
3 660	9 972	1.00	0 00	BrD ATOM	1863	CB	LYS	111	8 989	-
5 308	10 972	1 00	0.00	BrD ATOM	1864	HB1	LYS	111	9 742	-
5.373	11 743	1 00	0 00	BrD ATOM	1865	HB2	LYS	111	8.661	-
6 304	10 718	1.00	0 00	BrD ATOM	1866	CG	LYS	111	7 801	-
4 542	11.528	1.00	0 00	BrD ATOM	1867	HG1	LYS	111	7 127	-
4 304	10 718	1 00	0.00	BrD ATOM	1868	HG2	LYS	111	7 293	-
5.162	12 252	1 00	0.00	BrD ATOM	1869	CD	LYS	111	8 237	-
3 252	12 203	1 00	0.00	BrD ATOM	1870	HD1	LYS	111	8 872	-
2 701	11 525	1 00	0.00	BrD ATOM	1871	HD2	LYS	111	7.361	-
2 666	12 437	1 00	0 00	BrD ATOM	1872	CE	LYS	111	9 006	-
3 527	13.485	1.00	0 00	BrD ATOM	1873	HE1	LYS	111	10 044	-
3 698	13.239	1 00	0 00	BrD ATOM	1874	HE2	LYS	111	8 597	-
4.411	13 952	1 00	0 00	BrD ATOM	1875	NZ	LYS	111	8 916	-
2 389	14 442	1 00	0 00	BrD ATOM	1876	HZ1	LYS	111	9.335	-
2.656	15 356	1 00	0 00	BrD ATOM	1877	HZ2	LYS	111	7.921	-
2.127	14 593	1 00	0.00	BrD ATOM	1878	HZ3	LYS	111	9 428	-
1.565	14 066	1 00	0.00	BrD ATOM	1879	C	LYS	111	10 828	-
5 465	9 289	1.00	0.00	BrD ATOM	1880	O	LYS	111	11 964	-
5 112	9 607	1 00	0 00	BrD ATOM	1881	N	GLU	112	10 585	-
6 549	8 561	1 00	0 00	BrD ATOM	1882	HN	GLU	112	9 658	-
6 780	8 344	1 00	0 00	BrD ATOM	1883	CA	GLU	112	11 662	-
7.407	8 085	1 00	0 00	BrD ATOM	1884	HA	GLU	112	12 330	-
7.588	8.914	1 00	0 00	BrD ATOM	1885	CB	GLU	112	11.098	-
8.745	7 600	1 00	0 00	BrD ATOM	1886	HB1	GLU	112	10 589	-
8.589	6 661	1.00	0.00	BrD ATOM	1887	HB2	GLU	112	11 917	-
9.432	7 445	1 00	0 00	BrD ATOM	1888	CG	GLU	112	10 120	-
9 383	8 573	1 00	0 00	BrD ATOM	1889	HG1	GLU	112	10 678	-
9.856	9 367	1 00	0.00	BrD ATOM	1890	HG2	GLU	112	9 489	-
8 611	8 987	1 00	0 00	BrD ATOM	1891	CD	GLU	112	9 240	-
10.425	7 912	1 00	0.00	BrD ATOM	1892	OE1	GLU	112	9 625	-
10.932	6 837	1.00	0 00	BrD ATOM	1893	OE2	GLU	112	8 165	-
10.734	8 468	1 00	0.00	BrD ATOM	1894	C	GLU	112	12.447	-
6 739	6.960	1.00	0 00	BrD ATOM	1895	O	GLU	112	13 583	-
7 120	6 677	1 00	0.00	BrD ATOM	1896	N	ALA	113	11 840	-
5.744	6 318	1 00	0.00	BrD ATOM	1897	HN	ALA	113	10 932	-
5.486	6 579	1 00	0.00	BrD ATOM	1898	CA	ALA	113	12 492	-
5 046	5 216	1 00	0.00	BrD ATOM	1899	HA	ALA	113	13 355	-
5 620	4 936	1.00	0 00	BrD ATOM	1900	CB	ALA	113	11 573	-
4 989	4 008	1 00	0 00	BrD ATOM	1901	HB1	ALA	113	11 649	-
5 914	3 455	1.00	0 00	BrD ATOM	1902	HB2	ALA	113	11 865	-
4 166	3 373	1 00	0 00	BrD ATOM	1903	HB3	ALA	113	10.554	-
4.848	4 336	1 00	0.00	BrD ATOM	1904	C	ALA	113	12.953	-
3.645	5 624	1 00	0.00	BrD ATOM	1905	O	ALA	113	13 778	-
3.035	4 943	1 00	0.00	BrD ATOM	1906	N	GLY	114	12 435	-
3.146	6.743	1.00	0 00	BrD ATOM	1907	HN	GLY	114	11 790	-
3.678	7.255	1.00	0 00	BrD ATOM	1908	CA	GLY	114	12 833	-
1 836	7 229	1 00	0 00	BrD ATOM	1909	HA1	GLY	114	12.506	-
1 732	8 253	1 00	0 00	BrD ATOM	1910	HA2	GLY	114	13.911	-
1 769	7 200	1 00	0.00	BrD ATOM	1911	C	GLY	114	12 252	-
0.695	6 414	1 00	0.00	BrD ATOM	1912	O	GLY	114	12 991	
0.085	5 813	1 00	0.00	BrD ATOM	1913	N	LEU	115	10 927	-
0 590	6 405	1 00	0.00	BrD ATOM	1914	HN	LEU	115	10 398	-
1.231	6 921	1 00	0 00	BrD ATOM	1915	CA	LEU	115	10 244	
0.482	5 683	1 00	0.00	BrD ATOM	1916	HA	LEU	115	10.991	
1.195	5 369	1 00	0 00	BrD ATOM	1917	CB	LEU	115	9.523	-
0.066	4 442	1 00	0 00	BrD ATOM	1918	HB1	LEU	115	8.622	-
0 563	4 768	1.00	0 00	BrD ATOM	1919	HB2	LEU	115	9.240	
0.773	3.824	1.00	0.00	BrD ATOM	1920	CG	LEU	115	10 312	-
1 047	3 570	1 00	0.00	BrD ATOM	1921	HG	LEU	115	9 929	-
1.000	2 565	1 00	0.00	BrD ATOM	1922	CD1	LEU	115	10.120	-
2.469	4.061	1.00	0.00	BrD ATOM	1923	HD11	LEU	115	10 216	-
3 149	3 228	1 00	0.00	BrD ATOM	1924	HD12	LEU	115	9 137	-
2 571	4 493	1 00	0 00	BrD ATOM	1925	HD13	LEU	115	10 868	-
2.699	4 804	1.00	0.00	BrD ATOM	1926	CD2	LEU	115	11.790	-
0 683	3 517	1 00	0 00	BrD ATOM	1927	HD21	LEU	115	12.358	-
1.397	4 094	1 00	0.00	BrD ATOM	1928	HD22	LEU	115	11.932	
0.306	3 924	1 00	0 00	BrD ATOM	1929	HD23	LEU	115	12 127	-
0.701	2 491	1 00	0.00	BrD ATOM	1930	C	LEU	115	9.246	
1.193	6 603	1.00	0.00	BrD ATOM	1931	O	LEU	115	9.407	
1.183	7.823	1 00	0.00	BrD ATOM	1932	N	ILE	116	8 209	
1.801	6.018	1 00	0.00	BrD ATOM	1933	HN	ILE	116	8.131	
1.787	5 043	1 00	0.00	BrD ATOM	1934	CA	ILE	116	7 196	
2.518	6 794	1 00	0 00	BrD ATOM	1935	HA	ILE	116	7 614	
3.470	7 083	1 00	0 00	BrD ATOM	1936	CB	ILE	116	5 930	
2.786	5.956	1.00	0.00	BrD ATOM	1937	HB	ILE	116	5 183	
3.218	6 605	1.00	0.00	BrD ATOM	1938	CG1	ILE	116	5 388	
1 480	5.367	1.00	0.00	BrD ATOM	1939	HG11	ILE	116	4 697	
1 713	4 570	1 00	0.00	BrD ATOM	1940	HG12	ILE	116	6 209	
0 904	4 968	1.00	0 00	BrD ATOM	1941	CG2	ILE	116	6.228	
3 786	4 850	1 00	0.00	BrD ATOM	1942	HG21	ILE	116	5 309	
4 261	4 538	1.00	0.00	BrD ATOM	1943	HG22	ILE	116	6.671	
3 271	4 010	1 00	0.00	BrD ATOM	1944	HG23	ILE	116	6 914	

4.534	5.217	1.00	0.00	BrD ATOM	1945	CD1 ILE	116	4.662
0 615	6 373	1 00	0.00	BrD ATOM	1946	HD11 ILE	116	3.870
0.073	5.875	1 00	0.00	BrD ATOM	1947	HD12 ILE	116	4 240
1 238	7 147	1 00	0.00	BrD ATOM	1948	HD13 ILE	116	5.356
0 086	6 812	1 00	0 00	BrD ATOM	1949	C ILE	116	6 802
1 751	8 053	1 00	0.00	BrD ATOM	1950	O ILE	116	7.024
0 544	8 154	1 00	0 00	BrD ATOM	1951	N ASP	117	6 222
2 465	9 014	1.00	0 00	BrD ATOM	1952	HN ASP	117	6 079
3 424	8 874	1.00	0 00	BrD ATOM	1953	CA ASP	117	5 805
1 862	10.275	1 00	0 00	BrD ATOM	1954	HA ASP	117	5 197
2 585	10 798	1.00	0.00	BrD ATOM	1955	CB ASP	117	4.967
0 609	10 013	1 00	0.00	BrD ATOM	1956	HB1 ASP	117	5 564
0 267	10 220	1 00	0 00	BrD ATOM	1957	HB2 ASP	117	4 664
0 596	8 976	1 00	0.00	BrD ATOM	1958	CG ASP	117	3.722
0 555	10 876	1 00	0 00	BrD ATOM	1959	OD1 ASP	117	2 897
1 488	10 787	1 00	0 00	BrD ATOM	1960	OD2 ASP	117	3.572
0 421	11 641	1 00	0 00	BrD ATOM	1961	C ASP	117	7 006
1.506	11 154	1 00	0 00	BrD ATOM	1962	O ASP	117	6 846
0 892	12 209	1 00	0 00	BrD ATOM	1963	N LYS	118	8 206
1 897	10 725	1 00	0 00	BrD ATOM	1964	HN LYS	118	8 282
2 384	9 879	1 00	0.00	BrD ATOM	1965	CA LYS	118	9 416
1 613	11 488	1 00	0 00	BrD ATOM	1966	HA LYS	118	10 248
2 063	10 968	1 00	0.00	BrD ATOM	1967	CB LYS	118	9 315
2.220	12 889	1 00	0.00	BrD ATOM	1968	HB1 LYS	118	8 636
1 624	13 480	1 00	0.00	BrD ATOM	1969	HB2 LYS	118	10.292
2 199	13 349	1 00	0 00	BrD ATOM	1970	CG LYS	118	8 818
3 656	12 895	1 00	0 00	BrD ATOM	1971	HG1 LYS	118	7 921
3 719	12 296	1 00	0 00	BrD ATOM	1972	HG2 LYS	118	8.595
3 946	13 911	1 00	0 00	BrD ATOM	1973	CD LYS	118	9 857
4 608	12 327	1 00	0 00	BrD ATOM	1974	HD1 LYS	118	10 477
4 972	13 133	1.00	0.00	BrD ATOM	1975	HD2 LYS	118	10 468
4 075	11 613	1 00	0.00	BrD ATOM	1976	CE LYS	118	9.208
5 794	11 631	1.00	0 00	BrD ATOM	1977	HE1 LYS	118	8 502
5 425	10 902	1 00	0 00	BrD ATOM	1978	HE2 LYS	118	8.687
6.386	12 269	1 00	0 00	BrD ATOM	1979	NZ LYS	118	10 212
6 652	10 943	1 00	0 00	BrD ATOM	1980	HZ1 LYS	118	11 163
6 458	11 316	1 00	0 00	BrD ATOM	1981	HZ2 LYS	118	9 989
7 656	11 096	1 00	0 00	BrD ATOM	1982	HZ3 LYS	118	10.206
6 459	9 921	1 00	0 00	BrD ATOM	1983	C LYS	118	9 657
0.110	11 591	1 00	0 00	BrD ATOM	1984	OT1 LYS	118	9 047
0 641	10 802	1 00	0 00	BrD ATOM	1985	OT2 LYS	118	10.454
0 302	12 459	1 00	0 00	BrD END				

Structure-based sequence homology alignment of bromodomains

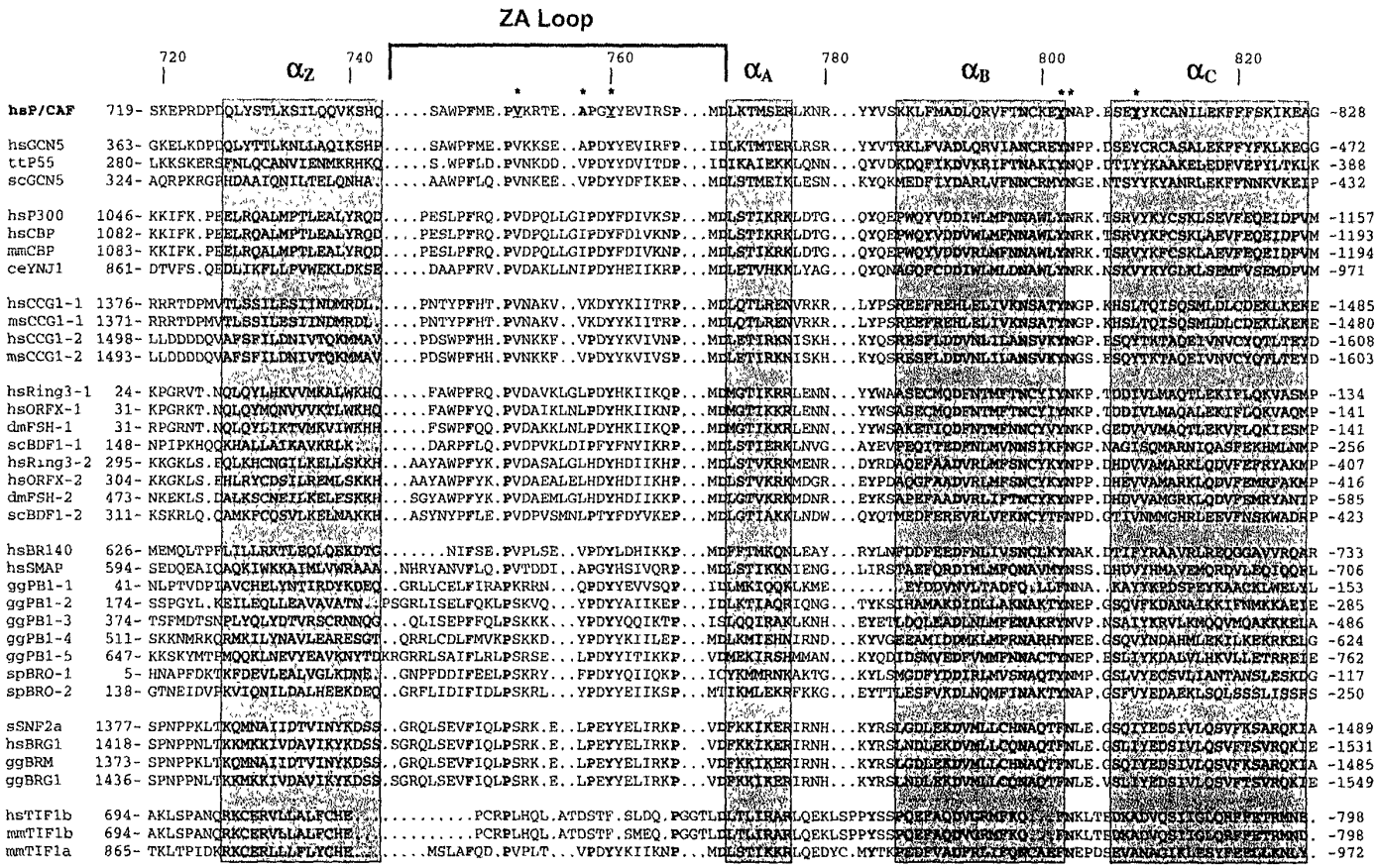

Figure 1

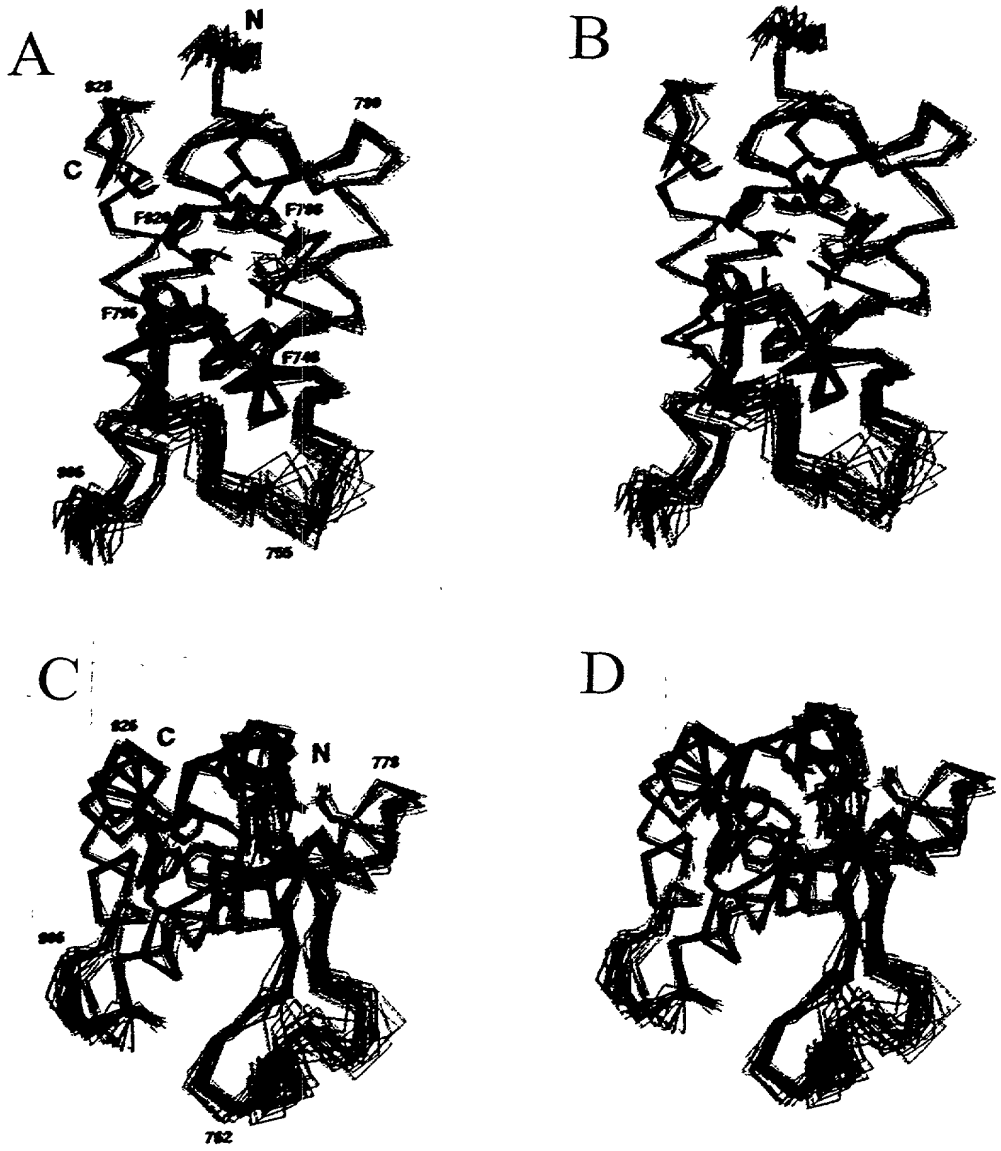

Figure 2A-2D

Three-Dimensional Structure of the P/CAF Bromodomain

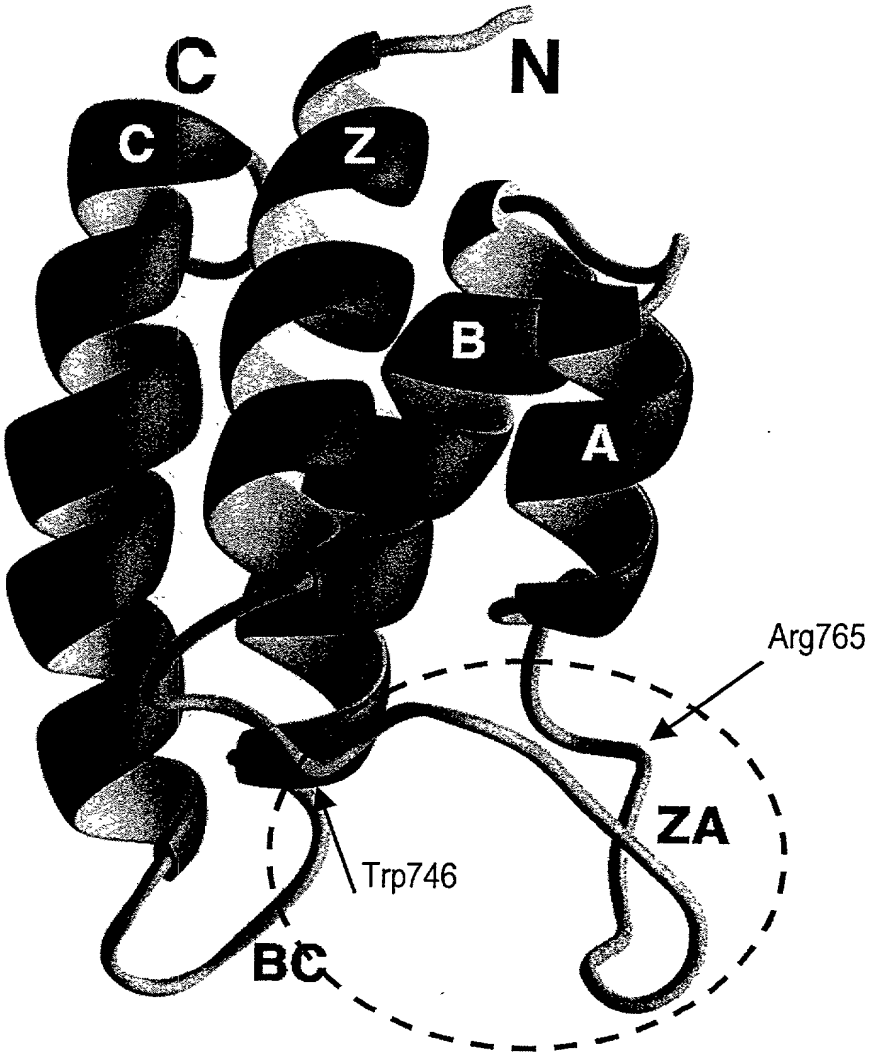

Figure 2E

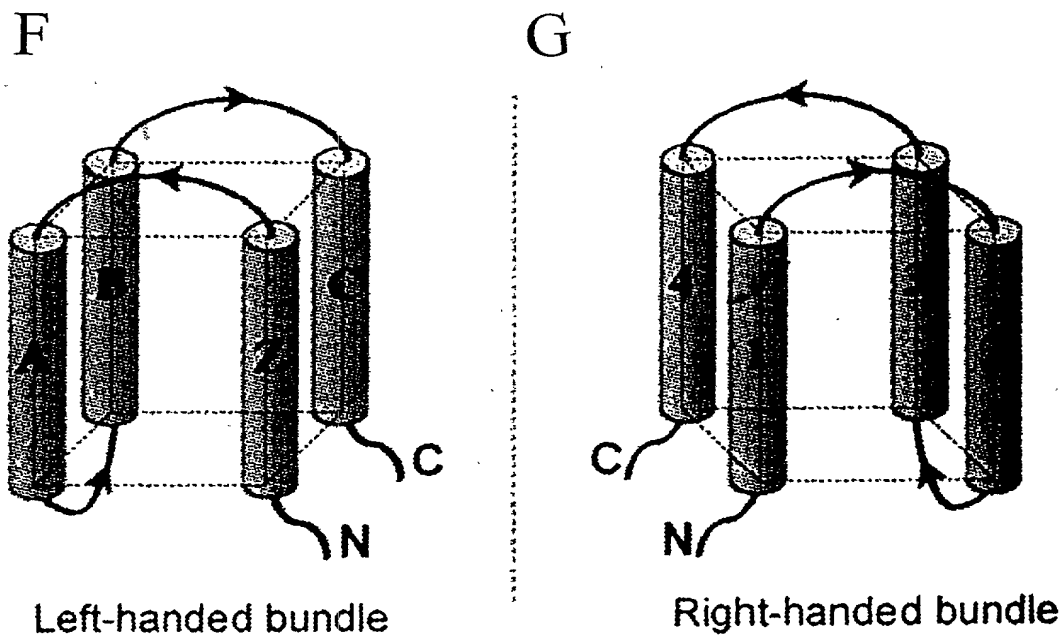

Figure 2F-2G

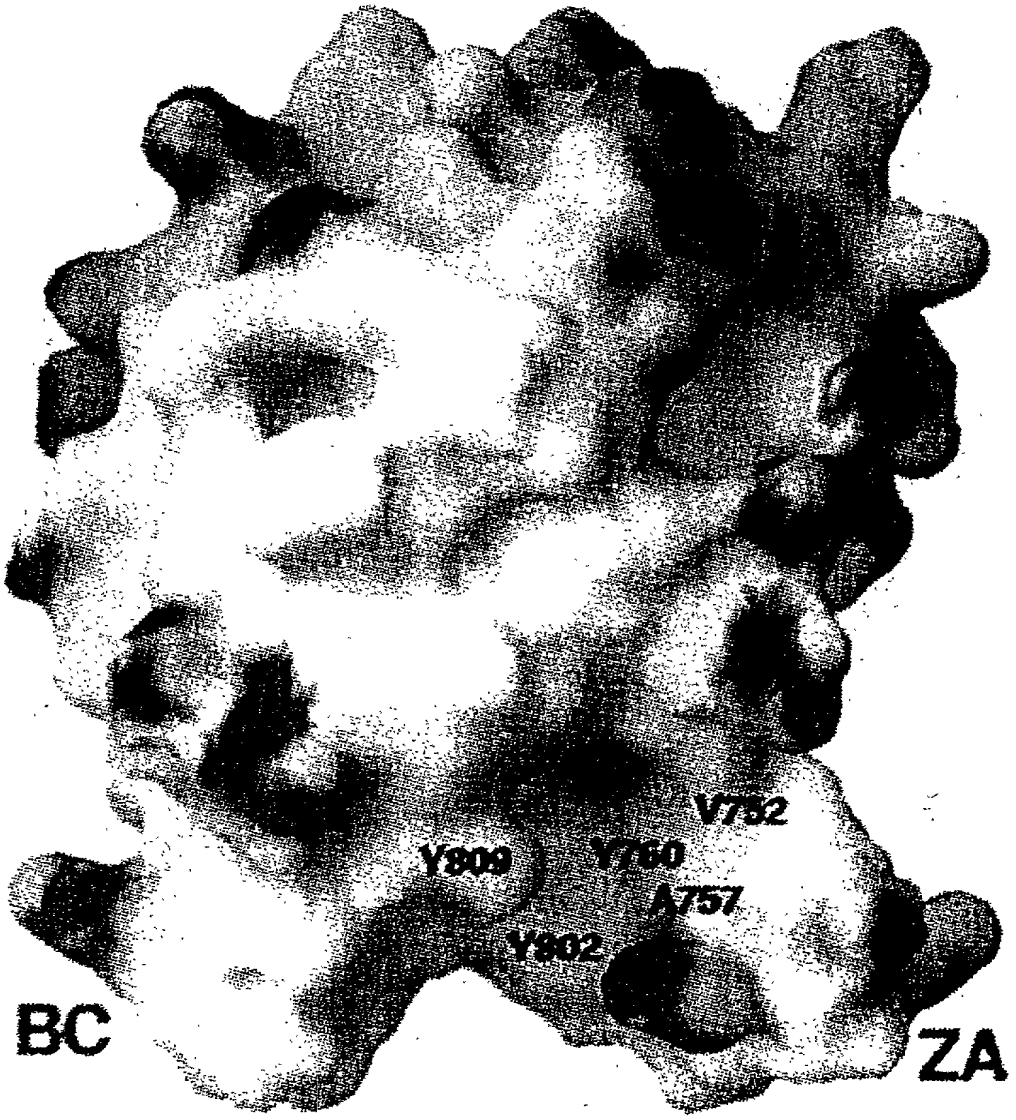

Figure 2H

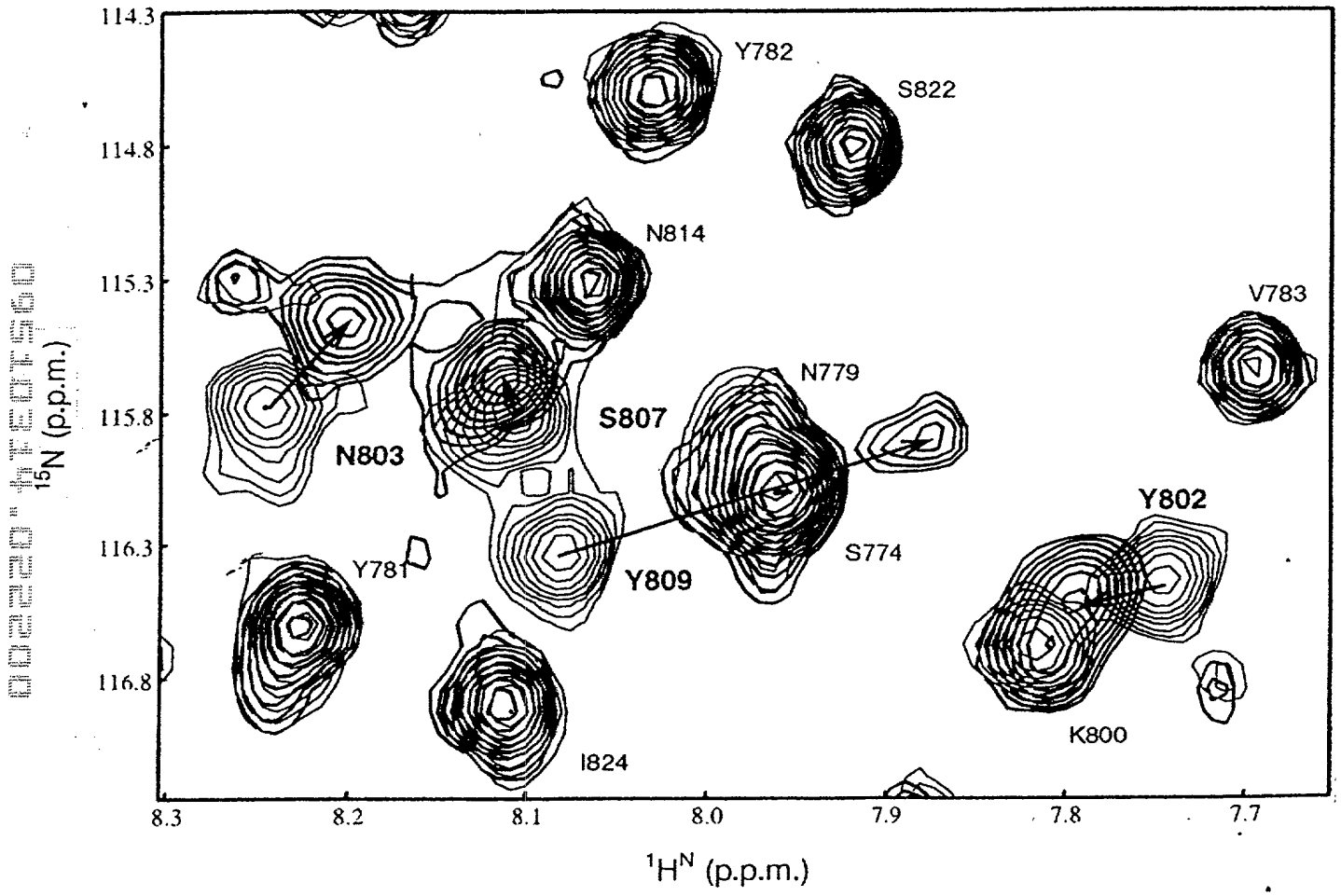
114.3
114.8
115.3
115.8
116.3
116.8
^{15}N (p.p.m.)
Y782
S822
N814
V783
N779
S807
N803
Y802
S774
Y781
Y809
K800
I824
8.3
8.2
8.1
8.0
7.9
7.8
7.7
^{1}H^{N} (p.p.m.)

Figure 3A

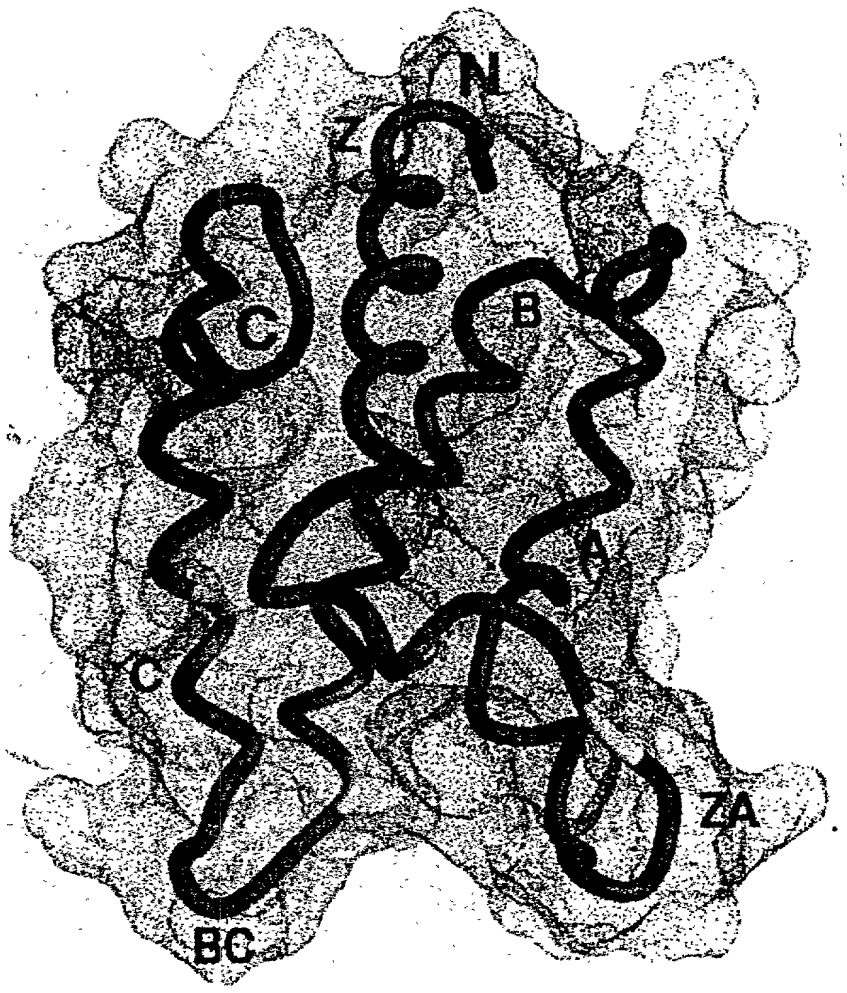

Figure 3B

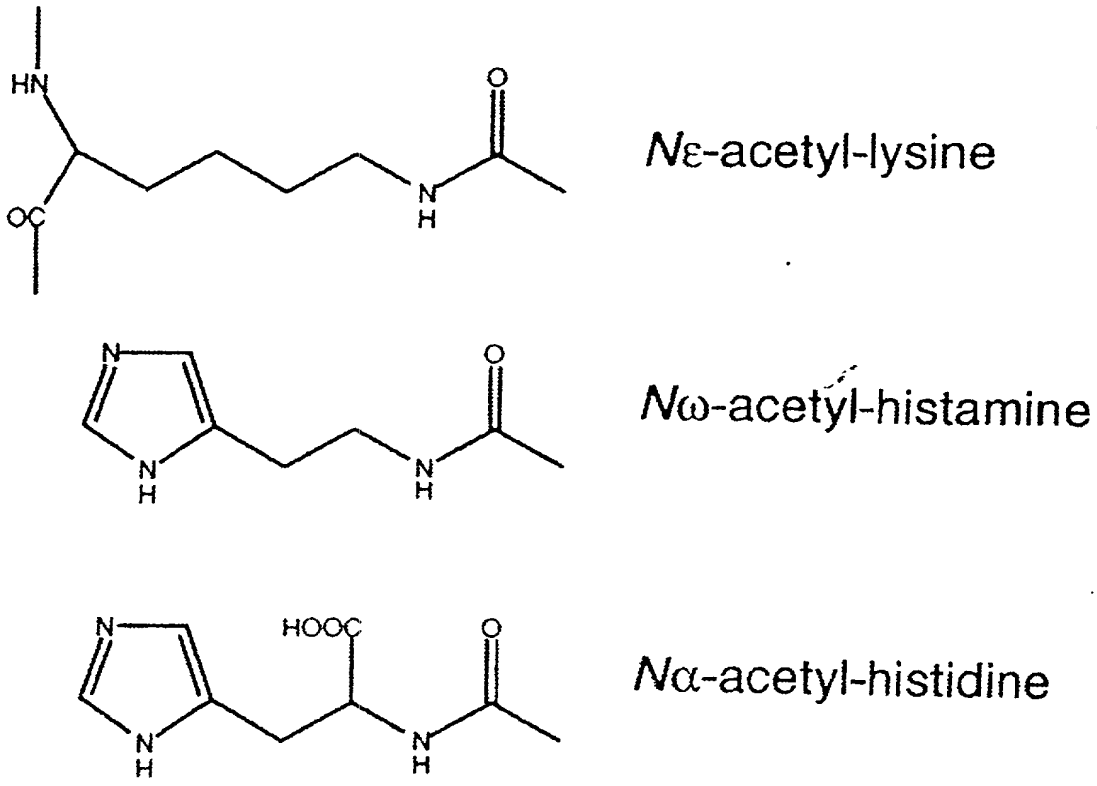
HN
O
OC
N
H
Nε-acetyl-lysine
N
O
N
H
N
H
Nω-acetyl-histamine
N
HOOC
O
N
H
N
H
Nα-acetyl-histidine

Figure 3C

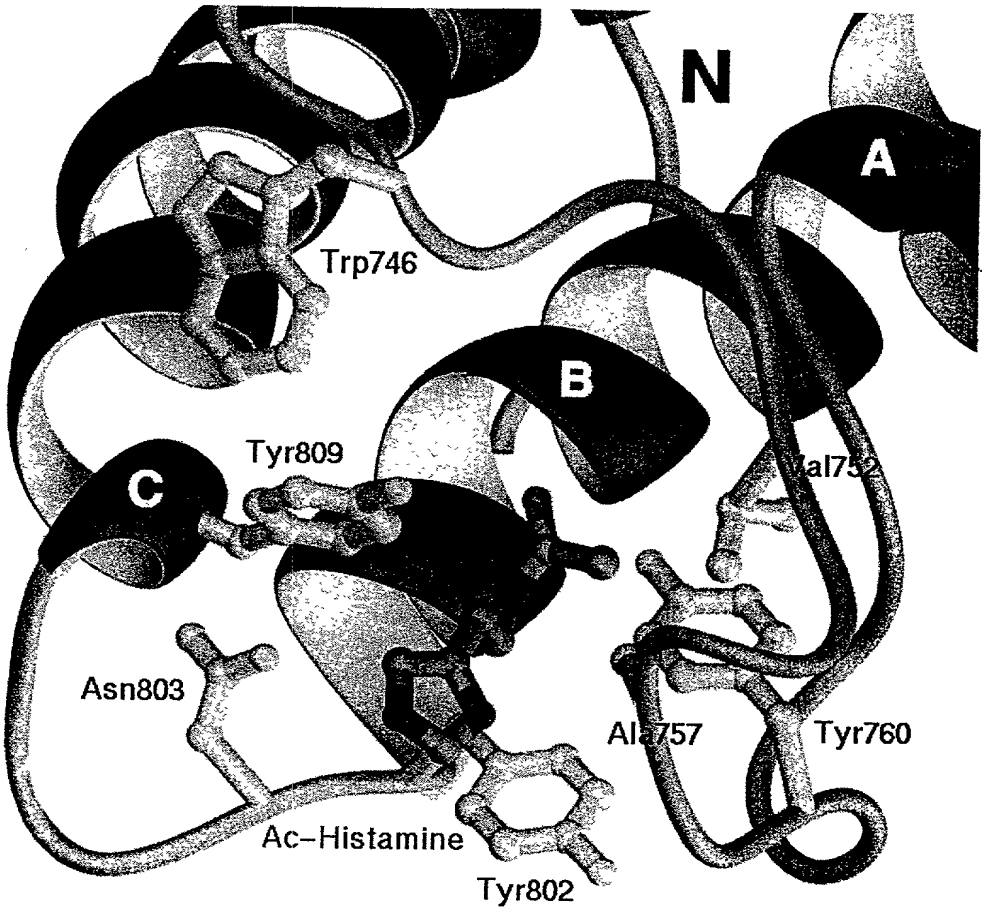

Figure 4

Attorney Docket No:2459-1-003

DECLARATION AND POWER OF ATTORNEY FOR PATENT APPLICATION

As below named inventors, we hereby declare that:

Our residence, post office address and citizenship are as stated below under our names.

We believe that we are the original, first and joint inventors of the subject matter which is claimed and for which a patent is sought on the invention entitled

METHODS OF IDENTIFYING MODULATORS OF BROMODOMAINS

the Specification of which

[X] is attached hereto

[ ] was filed on _____
as Application Serial No. _____
and was amended on _____ (if applicable).

We hereby state that we have reviewed and understand the contents of the above-identified Specification, including the claims, as amended by any amendment referred to above.

We acknowledge the duty to disclose information which is material to the examination of this application in accordance with Title 37, Code of Federal Regulations, 1.56(a).

We hereby claim foreign priority benefits under Title 35, United States Code, §119 of any provisional application filed in the United States in accordance with 35 U.S.C. §1.119(e), or any application for patent that has been converted to a Provisional Application within one (1) year of its filing date, or any foreign application(s) for patent or inventor's certificate listed below and have also identified below any foreign application for patent or inventor's certificate having a filing date before that of the application on which priority is claimed.

PRIOR FILED APPLICATION(S)			
APPLICATION NUMBER	COUNTRY	(DAY/MONTH/YEAR FILED)	PRIORITY CLAIMED

We hereby claim the benefit under Title 35, United States Code, §120 of any United States application listed below, and, insofar as the subject matter of each of the claims of this application is not disclosed in any prior United States application in the manner provided by the first paragraph of Title 35, United States Code, §112, I acknowledge the duty to disclose material information as defined in Title 37, Code of Federal Regulations, §1.56(a), which occurred between the filing date of the prior application and the national or PCT international filing date of this application:

Attorney Docket No:2459-1-003

APPLICATION NO.	FILING DATE (DAY/MONTH/YEAR)	STATUS - PATENTED, PENDING, ABANDONED

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We hereby declare that all statements made herein of my own knowledge are true and that all statements made on information and belief are believed to be true; and further, that these statements were made with the knowledge that willful false statements and the like so made are punishable by fine or imprisonment, or both, under Section 1001 of Title 18 of the United States Code and that such willful false statements may jeopardize the validity of the application or any patent issued thereon.

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SIGNATURE OF INVENTOR _____

DATE _____

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DATE _____

SEQUENCE LISTING

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Aggarnal, Aneel K

<120> METHODS OF IDENTIFYING MODULATORS OF BROMODOMAINS

<130> 2459-1-003

<140> UNASSIGNED
<141> 2000-02-22

<160> 44

<170> PatentIn Ver. 2.0

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<211> 832
<212> PRT
<213> Homo sapiens

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Gly Ala Gly Ala Gly Pro Gly Ala Leu Pro Pro Gln Pro Ala Ala Leu
20 25 30

Pro Pro Ala Pro Pro Gln Gly Ser Pro Cys Ala Ala Ala Ala Gly Gly
35 40 45

Ser Gly Ala Cys Gly Pro Ala Thr Ala Val Ala Ala Ala Gly Thr Ala
50 55 60

Glu Gly Pro Gly Gly Gly Gly Ser Ala Arg Ile Ala Val Lys Lys Ala
65 70 75 80

Gln Leu Arg Ser Ala Pro Arg Ala Lys Lys Leu Glu Lys Leu Gly Val

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                85                  90                  95

Tyr Ser Ala Cys Lys Ala Glu Glu Ser Cys Lys Cys Asn Gly Trp Lys
            100                 105                 110

Asn Pro Asn Pro Ser Pro Thr Pro Pro Arg Ala Asp Leu Gln Gln Ile
        115                 120                 125

Ile Val Ser Leu Thr Glu Ser Cys Arg Ser Cys Ser His Ala Leu Ala
    130                 135                 140

Ala His Val Ser His Leu Glu Asn Val Ser Glu Glu Glu Met Asn Arg
145                 150                 155                 160

Leu Leu Gly Ile Val Leu Asp Val Glu Tyr Leu Phe Thr Cys Val His
                165                 170                 175

Lys Glu Glu Asp Ala Asp Thr Lys Gln Val Tyr Phe Tyr Leu Phe Lys
            180                 185                 190

Leu Leu Arg Lys Ser Ile Leu Gln Arg Gly Lys Pro Val Val Glu Gly
        195                 200                 205

Ser Leu Glu Lys Lys Pro Pro Phe Glu Lys Pro Ser Ile Glu Gln Gly
    210                 215                 220

Val Asn Asn Phe Val Gln Tyr Lys Phe Ser His Leu Pro Ala Lys Glu
225                 230                 235                 240

Arg Gln Thr Ile Val Glu Leu Ala Lys Met Phe Leu Asn Arg Ile Asn
                245                 250                 255

Tyr Trp His Leu Glu Ala Pro Ser Gln Arg Arg Leu Arg Ser Pro Asn
            260                 265                 270

Asp Asp Ile Ser Gly Tyr Lys Glu Asn Tyr Thr Arg Trp Leu Cys Tyr
        275                 280                 285

Cys Asn Val Pro Gln Phe Cys Asp Ser Leu Pro Arg Tyr Glu Thr Thr
    290                 295                 300

Gln Val Phe Gly Arg Thr Leu Leu Arg Ser Val Phe Thr Val Met Arg
305                 310                 315                 320

Arg Gln Leu Leu Glu Gln Ala Arg Gln Glu Lys Asp Lys Leu Pro Leu
                325                 330                 335

Glu Lys Arg Thr Leu Ile Leu Thr His Phe Pro Lys Phe Leu Ser Met
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            340                 345                 350

Leu Glu Glu Glu Val Tyr Ser Gln Asn Ser Pro Ile Trp Asp Gln Asp
        355                 360                 365

Phe Leu Ser Ala Ser Ser Arg Thr Ser Gln Leu Gly Ile Gln Thr Val
    370                 375                 380

Ile Asn Pro Pro Pro Val Ala Gly Thr Ile Ser Tyr Asn Ser Thr Ser
385                 390                 395                 400

Ser Ser Leu Glu Gln Pro Asn Ala Gly Ser Ser Ser Pro Ala Cys Lys
                405                 410                 415

Ala Ser Ser Gly Leu Glu Ala Asn Pro Gly Glu Lys Arg Lys Met Thr
            420                 425                 430

Asp Ser His Val Leu Glu Glu Ala Lys Lys Pro Arg Val Met Gly Asp
        435                 440                 445

Ile Pro Met Glu Leu Ile Asn Glu Val Met Ser Thr Ile Thr Asp Pro
    450                 455                 460

Ala Ala Met Leu Gly Pro Glu Thr Asn Phe Leu Ser Ala His Ser Ala
465                 470                 475                 480

Arg Asp Glu Ala Ala Arg Leu Glu Glu Arg Arg Gly Val Ile Glu Phe
                485                 490                 495

His Val Val Gly Asn Ser Leu Asn Gln Lys Pro Asn Lys Lys Ile Leu
            500                 505                 510

Met Trp Leu Val Gly Leu Gln Asn Val Phe Ser His Gln Leu Pro Arg
        515                 520                 525

Met Pro Lys Glu Tyr Ile Thr Arg Leu Val Phe Asp Pro Lys His Lys
    530                 535                 540

Thr Leu Ala Leu Ile Lys Asp Gly Arg Val Ile Gly Gly Ile Cys Phe
545                 550                 555                 560

Arg Met Phe Pro Ser Gln Gly Phe Thr Glu Ile Val Phe Cys Ala Val
                565                 570                 575

Thr Ser Asn Glu Gln Val Lys Gly Tyr Gly Thr His Leu Met Asn His
            580                 585                 590

Leu Lys Glu Tyr His Ile Lys His Asp Ile Leu Asn Phe Leu Thr Tyr
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595 600 605

Ala Asp Glu Tyr Ala Ile Gly Tyr Phe Lys Lys Gln Gly Phe Ser Lys
610 615 620

Glu Ile Lys Ile Pro Lys Thr Lys Tyr Val Gly Tyr Ile Lys Asp Tyr
625 630 635 640

Glu Gly Ala Thr Leu Met Gly Cys Glu Leu Asn Pro Arg Ile Pro Tyr
645 650 655

Thr Glu Phe Ser Val Ile Ile Lys Lys Gln Lys Glu Ile Ile Lys Lys
660 665 670

Leu Ile Glu Arg Lys Gln Ala Gln Ile Arg Lys Val Tyr Pro Gly Leu
675 680 685

Ser Cys Phe Lys Asp Gly Val Arg Gln Ile Pro Ile Glu Ser Ile Pro
690 695 700

Gly Ile Arg Glu Thr Gly Trp Lys Pro Ser Gly Lys Glu Lys Ser Lys
705 710 715 720

Glu Pro Arg Asp Pro Asp Gln Leu Tyr Ser Thr Leu Lys Ser Ile Leu
725 730 735

Gln Gln Val Lys Ser His Gln Ser Ala Trp Pro Phe Met Glu Pro Val
740 745 750

Lys Arg Thr Glu Ala Pro Gly Tyr Tyr Glu Val Ile Arg Phe Pro Met
755 760 765

Asp Leu Lys Thr Met Ser Glu Arg Leu Lys Asn Arg Tyr Tyr Val Ser
770 775 780

Lys Lys Leu Phe Met Ala Asp Leu Gln Arg Val Phe Thr Asn Cys Lys
785 790 795 800

Glu Tyr Asn Ala Ala Glu Ser Glu Tyr Tyr Lys Cys Ala Asn Ile Leu
805 810 815

Glu Lys Phe Phe Phe Ser Lys Ile Lys Glu Ala Gly Leu Ile Asp Lys
820 825 830

<210> 3
<211> 12
<212> PRT
<213> Artificial Sequence

<220>
<223> Description of Artificial Sequence: peptide

<220>
<221> VARIANT
<222> (2)
<223> It represents 2 to 3 undesignated amino acids.
They can be any amino acids.

<220>
<221> VARIANT
<222> (4)
<223> It represents 5 to 8 undesignated amino acids.
They can be any amino acids.

<220>
<221> VARIANT
<222> (6)
<223> It represents one undesignated amino acid. It can
be any amino acid.

<220>
<221> VARIANT
<222> (9)
<223> It represents 5 undesignated amino acids. They can
be any amino acids.

<220>
<221> VARIANT
<222> (5)
<223> It can be any amino acid from the group of: P, K,
or H.

<220>
<221> VARIANT
<222> (8)
<223> It can be any amino acid from the group of: Y, F,
or H.

<220>
<221> VARIANT
<222> (11)
<223> It can be any amino acid from the group of: M, I,

or V.

<400> 3
Phe Xaa Pro Xaa Xaa Xaa Tyr Xaa Xaa Pro Xaa Asp
1 5 10

<210> 4
<211> 12
<212> PRT
<213> Artificial Sequence

<220>
<223> Description of Artificial Sequence: peptide

<220>
<221> SITE
<222> (6)
<223> It is acetyl-lysine.

<400> 4
Ile Ser Tyr Gly Arg Xaa Lys Arg Arg Gln Arg Arg
1 5 10

<210> 5
<211> 14
<212> PRT
<213> Artificial Sequence

<220>
<223> Description of Artificial Sequence: peptide

<220>
<221> SITE
<222> (8)
<223> It is acetyl-lysine.

<400> 5
Ala Arg Lys Ser Thr Gly Gly Xaa Ala Pro Arg Lys Gln Leu
1 5 10

<210> 6
<211> 14
<212> PRT
<213> Artificial Sequence

<220>
<223> Description of Artificial Sequence: peptide

<220>
<221> SITE
<222> (8)
<223> It is acetyl-lysine.

<400> 6
Gln Ser Thr Ser Arg His Lys Xaa Leu Met Phe Lys Thr Glu
1 5 10

<210> 7
<211> 110
<212> PRT
<213> Homo sapiens

<400> 7
Ser Lys Glu Pro Arg Asp Pro Asp Gln Leu Tyr Ser Thr Leu Lys Ser
1 5 10 15

Ile Leu Gln Gln Val Lys Ser His Gln Ser Ala Trp Pro Phe Met Glu
20 25 30

Pro Val Lys Arg Thr Glu Ala Pro Gly Tyr Tyr Glu Val Ile Arg Ser
35 40 45

Pro Met Asp Leu Lys Thr Met Ser Glu Arg Leu Lys Asn Arg Tyr Tyr
50 55 60

Val Ser Lys Lys Leu Phe Met Ala Asp Leu Gln Arg Val Phe Thr Asn
65 70 75 80

Cys Lys Glu Tyr Asn Ala Pro Glu Ser Glu Tyr Tyr Lys Cys Ala Asn
85 90 95

Ile Leu Glu Lys Phe Phe Phe Ser Lys Ile Lys Glu Ala Gly
100 105 110

<210> 8
<211> 110
<212> PRT
<213> Homo sapiens

<400> 8
Gly Lys Glu Leu Lys Asp Pro Asp Gln Leu Tyr Thr Thr Leu Lys Asn

1 5 10 15

Leu Leu Ala Gln Ile Lys Ser His Pro Ser Ala Trp Pro Phe Met Glu
20 25 30

Pro Val Lys Lys Ser Glu Ala Pro Asp Tyr Tyr Glu Val Ile Arg Phe
35 40 45

Pro Ile Asp Leu Lys Thr Met Thr Glu Arg Leu Arg Ser Arg Tyr Tyr
50 55 60

Val Thr Arg Lys Leu Phe Val Ala Asp Leu Gln Arg Val Ile Ala Asn
65 70 75 80

Cys Arg Glu Tyr Asn Pro Pro Asp Ser Glu Tyr Cys Arg Cys Ala Ser
85 90 95

Ala Leu Glu Lys Phe Phe Tyr Phe Lys Leu Lys Glu Gly Gly
100 105 110

<210> 9
<211> 109
<212> PRT
<213> Tetrahymena thermophila

<400> 9
Leu Lys Lys Ser Lys Glu Arg Ser Phe Asn Leu Gln Cys Ala Asn Val
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Ile Glu Asn Met Lys Arg His Lys Gln Ser Trp Pro Phe Leu Asp Pro
20 25 30

Val Asn Lys Asp Asp Val Pro Asp Tyr Tyr Asp Val Ile Thr Asp Pro
35 40 45

Ile Asp Ile Lys Ala Ile Glu Lys Lys Leu Gln Asn Asn Gln Tyr Val
50 55 60

Asp Lys Asp Gln Phe Ile Lys Asp Val Lys Arg Ile Phe Thr Asn Ala
65 70 75 80

Lys Ile Tyr Asn Gln Pro Asp Thr Ile Tyr Tyr Lys Ala Ala Lys Glu
85 90 95

Leu Glu Asp Phe Val Glu Pro Tyr Leu Thr Lys Leu Lys
100 105

<210> 10
<211> 109
<212> PRT
<213> Saccharomyces cerevisiae

<400> 10
Ala Gln Arg Pro Lys Arg Gly Pro His Asp Ala Ala Ile Gln Asn Ile
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Leu Thr Glu Leu Gln Asn His Ala Ala Ala Trp Pro Phe Leu Gln Pro
20 25 30

Val Asn Lys Glu Glu Val Pro Asp Tyr Tyr Asp Phe Ile Lys Glu Pro
35 40 45

Met Asp Leu Ser Thr Met Glu Ile Lys Leu Glu Ser Asn Lys Tyr Gln
50 55 60

Lys Met Glu Asp Phe Ile Tyr Asp Ala Arg Leu Val Phe Asn Asn Cys
65 70 75 80

Arg Met Tyr Asn Gly Glu Asn Thr Ser Tyr Tyr Lys Tyr Ala Asn Arg
85 90 95

Leu Glu Lys Phe Phe Asn Asn Lys Val Lys Glu Ile Pro
100 105

<210> 11
<211> 112
<212> PRT
<213> Homo sapiens

<400> 11
Lys Lys Ile Phe Lys Pro Glu Glu Leu Arg Gln Ala Leu Met Pro Thr
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Leu Glu Ala Leu Tyr Arg Gln Asp Pro Glu Ser Leu Pro Phe Arg Gln
20 25 30

Pro Val Asp Pro Gln Leu Leu Gly Ile Pro Asp Tyr Phe Asp Ile Val
35 40 45

Lys Ser Pro Met Asp Leu Ser Thr Ile Lys Arg Lys Leu Asp Thr Gly
50 55 60

Gln Tyr Gln Glu Pro Trp Gln Tyr Val Asp Asp Ile Trp Leu Met Phe

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 65                  70                  75                  80

Asn Asn Ala Trp Leu Tyr Asn Arg Lys Thr Ser Arg Val Tyr Lys Tyr
                 85                  90                  95

Cys Ser Lys Leu Ser Glu Val Phe Glu Gln Glu Ile Asp Pro Val Met
            100                 105                 110
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<210> 12
<211> 112
<212> PRT
<213> Homo sapiens

<400> 12

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Leu Glu Ala Leu Tyr Arg Gln Asp Pro Glu Ser Leu Pro Phe Arg Gln
             20                  25                  30

Pro Val Asp Pro Gln Leu Leu Gly Ile Pro Asp Tyr Phe Asp Ile Val
         35                  40                  45

Lys Asn Pro Met Asp Leu Ser Thr Ile Lys Arg Lys Leu Asp Thr Gly
     50                  55                  60

Gln Tyr Gln Glu Pro Trp Gln Tyr Val Asp Asp Val Trp Leu Met Phe
 65                  70                  75                  80

Asn Asn Ala Trp Leu Tyr Asn Arg Lys Thr Ser Arg Val Tyr Lys Phe
                 85                  90                  95

Cys Ser Lys Leu Ala Glu Val Phe Glu Gln Glu Ile Asp Pro Val Met
            100                 105                 110
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<210> 13
<211> 112
<212> PRT
<213> Mus musculus

<400> 13
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1 5 10 15

Leu Glu Ala Leu Tyr Arg Gln Asp Pro Glu Ser Leu Pro Phe Arg Gln
20 25 30

Pro Val Asp Pro Gln Leu Leu Gly Ile Pro Asp Tyr Phe Asp Ile Val
35 40 45

Lys Asn Pro Met Asp Leu Ser Thr Ile Lys Arg Lys Leu Asp Thr Gly
50 55 60

Gln Tyr Gln Glu Pro Trp Gln Tyr Val Asp Asp Val Arg Leu Met Phe
65 70 75 80

Asn Asn Ala Trp Leu Tyr Asn Arg Lys Thr Ser Arg Val Tyr Lys Phe
85 90 95

Cys Ser Lys Leu Ala Glu Val Phe Glu Gln Glu Ile Asp Pro Val Met
100 105 110

<210> 14
<211> 111
<212> PRT
<213> Caenorhabditis elegans

<400> 14
Asp Thr Val Phe Ser Gln Glu Asp Leu Ile Lys Phe Leu Leu Pro Val
1 5 10 15

Trp Glu Lys Leu Asp Lys Ser Glu Asp Ala Ala Pro Phe Arg Val Pro
20 25 30

Val Asp Ala Lys Leu Leu Asn Ile Pro Asp Tyr His Glu Ile Ile Lys
35 40 45

Arg Pro Met Asp Leu Glu Thr Val His Lys Lys Leu Tyr Ala Gly Gln
50 55 60

Tyr Gln Asn Ala Gly Gln Phe Cys Asp Asp Ile Trp Leu Met Leu Asp
65 70 75 80

Asn Ala Trp Leu Tyr Asn Arg Lys Asn Ser Lys Val Tyr Lys Tyr Gly

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                85                  90                  95

Leu Lys Leu Ser Glu Met Phe Val Ser Glu Met Asp Pro Val Met
            100                 105                 110


<210> 15
<211> 110
<212> PRT
<213> Homo sapiens

<400> 15
Arg Arg Arg Thr Asp Pro Met Val Thr Leu Ser Ser Ile Leu Glu Ser
  1               5                  10                  15

Ile Ile Asn Asp Met Arg Asp Leu Pro Asn Thr Tyr Pro Phe His Thr
             20                  25                  30

Pro Val Asn Ala Lys Val Val Lys Asp Tyr Tyr Lys Ile Ile Thr Arg
         35                  40                  45

Pro Met Asp Leu Gln Thr Leu Arg Glu Asn Val Arg Lys Arg Leu Tyr
     50                  55                  60

Pro Ser Arg Glu Glu Phe Arg Glu His Leu Glu Leu Ile Val Lys Asn
 65                  70                  75                  80

Ser Ala Thr Tyr Asn Gly Pro Lys His Ser Leu Thr Gln Ile Ser Gln
                85                  90                  95

Ser Met Leu Asp Leu Cys Asp Glu Lys Leu Lys Glu Lys Glu
            100                 105                 110


<210> 16
<211> 110
<212> PRT
<213> Mesocricetus auratus

<400> 16
Arg Arg Arg Thr Asp Pro Met Val Thr Leu Ser Ser Ile Leu Glu Ser
  1               5                  10                  15

Ile Ile Asn Asp Met Arg Asp Leu Pro Asn Thr Tyr Pro Phe His Thr
             20                  25                  30

Pro Val Asn Ala Lys Val Val Lys Asp Tyr Tyr Lys Ile Ile Thr Arg
         35                  40                  45
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Pro Met Asp Leu Gln Thr Leu Arg Glu Asn Val Arg Lys Arg Leu Tyr
     50                  55                  60

Pro Ser Arg Glu Glu Phe Arg Glu His Leu Glu Leu Ile Val Lys Asn
 65                  70                  75                  80

Ser Ala Thr Tyr Asn Gly Pro Lys His Ser Leu Thr Gln Ile Ser Gln
                 85                  90                  95

Ser Met Leu Asp Leu Cys Asp Glu Lys Leu Lys Glu Lys Glu
            100                 105                 110
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<210> 17
<211> 111
<212> PRT
<213> Homo sapiens

<400> 17

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Leu Leu Asp Asp Asp Asp Gln Val Ala Phe Ser Phe Ile Leu Asp Asn
  1               5                  10                  15

Ile Val Thr Gln Lys Met Met Ala Val Pro Asp Ser Trp Pro Phe His
             20                  25                  30

His Pro Val Asn Lys Lys Phe Val Pro Asp Tyr Tyr Lys Val Ile Val
         35                  40                  45

Asn Pro Met Asp Leu Glu Thr Ile Arg Lys Asn Ile Ser Lys His Lys
     50                  55                  60

Tyr Gln Ser Arg Glu Ser Phe Leu Asp Asp Val Asn Leu Ile Leu Ala
 65                  70                  75                  80

Asn Ser Val Lys Tyr Asn Gly Pro Glu Ser Gln Tyr Thr Lys Thr Ala
                 85                  90                  95

Gln Glu Ile Val Asn Val Cys Tyr Gln Thr Leu Thr Glu Tyr Asp
            100                 105                 110
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<210> 18
<211> 111
<212> PRT
<213> Mesocricetus auratus

<400> 18

Leu Leu Asp Asp Asp Asp Gln Val Ala Phe Ser Phe Ile Leu Asp Asn
1   5   10   15

Ile Val Thr Gln Lys Met Met Ala Val Pro Asp Ser Trp Pro Phe His
            20   25   30

His Pro Val Asn Lys Lys Phe Val Pro Asp Tyr Tyr Lys Val Ile Val
        35   40   45

Ser Pro Met Asp Leu Glu Thr Ile Arg Lys Asn Ile Ser Lys His Lys
    50   55   60

Tyr Gln Ser Arg Glu Ser Phe Leu Asp Asp Val Asn Leu Ile Leu Ala
65   70   75   80

Asn Ser Val Lys Tyr Asn Gly Ser Glu Ser Gln Tyr Thr Lys Thr Ala
                85   90   95

Gln Glu Ile Val Asn Val Cys Tyr Gln Thr Leu Thr Glu Tyr Asp
            100   105   110

<210> 19
<211> 111
<212> PRT
<213> Homo sapiens

<400> 19
Lys Pro Gly Arg Val Thr Asn Gln Leu Gln Tyr Leu His Lys Val Val
1   5   10   15

Met Lys Ala Leu Trp Lys His Gln Phe Ala Trp Pro Phe Arg Gln Pro
            20   25   30

Val Asp Ala Val Lys Leu Gly Leu Pro Asp Tyr His Lys Ile Ile Lys
        35   40   45

Gln Pro Met Asp Met Gly Thr Ile Lys Arg Arg Leu Glu Asn Asn Tyr
    50   55   60

Tyr Trp Ala Ala Ser Glu Cys Met Gln Asp Phe Asn Thr Met Phe Thr
65   70   75   80

Asn Cys Tyr Ile Tyr Asn Lys Pro Thr Asp Asp Ile Val Leu Met Ala
                85   90   95

Gln Thr Leu Glu Lys Ile Phe Leu Gln Lys Val Ala Ser Met Pro
            100   105   110

<210> 20
<211> 111
<212> PRT
<213> Homo sapiens

<400> 20
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1 5 10 15

Val Lys Thr Leu Trp Lys His Gln Phe Ala Trp Pro Phe Tyr Gln Pro
20 25 30

Val Asp Ala Ile Lys Leu Asn Leu Pro Asp Tyr His Lys Ile Ile Lys
35 40 45

Asn Pro Met Asp Met Gly Thr Ile Lys Lys Arg Leu Glu Asn Asn Tyr
50 55 60

Tyr Trp Ser Ala Ser Glu Cys Met Gln Asp Phe Asn Thr Met Phe Thr
65 70 75 80

Asn Cys Tyr Ile Tyr Asn Lys Pro Thr Asp Asp Ile Val Leu Met Ala
85 90 95

Gln Ala Leu Glu Lys Ile Phe Leu Gln Lys Val Ala Gln Met Pro
100 105 110

<210> 21
<211> 111
<212> PRT
<213> Drosophila melanogaster

<400> 21
Arg Pro Gly Arg Asn Thr Asn Gln Leu Gln Tyr Leu Ile Lys Thr Val
1 5 10 15

Met Lys Val Ile Trp Lys His His Phe Ser Trp Pro Phe Gln Gln Pro
20 25 30

Val Asp Ala Lys Lys Leu Asn Leu Pro Asp Tyr His Lys Ile Ile Lys
35 40 45

Gln Pro Met Asp Met Gly Thr Ile Lys Lys Arg Leu Glu Asn Asn Tyr
50 55 60

```
Tyr Trp Ser Ala Lys Glu Thr Ile Gln Asp Phe Asn Thr Met Phe Asn
 65                  70                  75                  80

Asn Cys Tyr Val Tyr Asn Lys Pro Gly Glu Asp Val Val Val Met Ala
                 85                  90                  95

Gln Thr Leu Glu Lys Val Phe Leu Gln Lys Ile Glu Ser Met Pro
            100                 105                 110


<210> 22
<211> 109
<212> PRT
<213> Saccharomyces cerevisiae

<400> 22
Asn Pro Ile Pro Lys His Gln Gln Lys His Ala Leu Leu Ala Ile Lys
  1               5                  10                  15

Ala Val Lys Arg Leu Lys Asp Ala Arg Pro Phe Leu Gln Pro Val Asp
             20                  25                  30

Pro Val Lys Leu Asp Ile Pro Phe Tyr Phe Asn Tyr Ile Lys Arg Pro
         35                  40                  45

Met Asp Leu Ser Thr Ile Glu Arg Lys Leu Asn Val Gly Ala Tyr Glu
     50                  55                  60

Val Pro Glu Gln Ile Thr Glu Asp Phe Asn Leu Met Val Asn Asn Ser
 65                  70                  75                  80

Ile Lys Phe Asn Gly Pro Asn Ala Gly Ile Ser Gln Met Ala Arg Asn
                 85                  90                  95

Ile Gln Ala Ser Phe Glu Lys His Met Leu Asn Met Pro
            100                 105


<210> 23
<211> 113
<212> PRT
<213> Homo sapiens

<400> 23
Lys Lys Gly Lys Leu Ser Glu Gln Leu Lys His Cys Asn Gly Ile Leu
  1               5                  10                  15

Lys Glu Leu Leu Ser Lys Lys His Ala Ala Tyr Ala Trp Pro Phe Tyr
```

```
            20                  25                  30

Lys Pro Val Asp Ala Ser Ala Leu Gly Leu His Asp Tyr His Asp Ile
         35                  40                  45

Ile Lys His Pro Met Asp Leu Ser Thr Val Lys Arg Lys Met Glu Asn
     50                  55                  60

Arg Asp Tyr Arg Asp Ala Gln Glu Phe Ala Ala Asp Val Arg Leu Met
 65                  70                  75                  80

Phe Ser Asn Cys Tyr Lys Tyr Asn Pro Pro Asp His Asp Val Val Ala
                 85                  90                  95

Met Ala Arg Lys Leu Gln Asp Val Phe Glu Phe Arg Tyr Ala Lys Met
            100                 105                 110

Pro
```


<210> 24
<211> 113
<212> PRT
<213> Homo sapiens

<400> 24

```
Lys Lys Gly Lys Leu Ser Glu His Leu Arg Tyr Cys Asp Ser Ile Leu
  1               5                  10                  15

Arg Glu Met Leu Ser Lys Lys His Ala Ala Tyr Ala Trp Pro Phe Tyr
             20                  25                  30

Lys Pro Val Asp Ala Glu Ala Leu Glu Leu His Asp Tyr His Asp Ile
         35                  40                  45

Ile Lys His Pro Met Asp Leu Ser Thr Val Lys Arg Lys Met Asp Gly
     50                  55                  60

Arg Glu Tyr Pro Asp Ala Gln Gly Phe Ala Ala Asp Val Arg Leu Met
 65                  70                  75                  80

Phe Ser Asn Cys Tyr Lys Tyr Asn Pro Pro Asp His Glu Val Val Ala
                 85                  90                  95

Met Ala Arg Lys Leu Gln Asp Val Phe Glu Met Arg Phe Ala Lys Met
            100                 105                 110
```

Pro

<210> 25
<211> 113
<212> PRT
<213> Drosophila melanogaster

<400> 25
Asn Lys Glu Lys Leu Ser Asp Ala Leu Lys Ser Cys Asn Glu Ile Leu
1 5 10 15

Lys Glu Leu Phe Ser Lys Lys His Ser Gly Tyr Ala Trp Pro Phe Tyr
20 25 30

Lys Pro Val Asp Ala Glu Met Leu Gly Leu His Asp Tyr His Asp Ile
35 40 45

Ile Lys Lys Pro Met Asp Leu Gly Thr Val Lys Arg Lys Met Asp Asn
50 55 60

Arg Glu Tyr Lys Ser Ala Pro Glu Phe Ala Ala Asp Val Arg Leu Ile
65 70 75 80

Phe Thr Asn Cys Tyr Lys Tyr Asn Pro Pro Asp His Asp Val Val Ala
85 90 95

Met Gly Arg Lys Leu Gln Asp Val Phe Glu Met Arg Tyr Ala Asn Ile
100 105 110

Pro

<210> 26
<211> 113
<212> PRT
<213> Saccharomyces cerevisiae

<400> 26
Lys Ser Lys Arg Leu Gln Gln Ala Met Lys Phe Cys Gln Ser Val Leu
1 5 10 15

Lys Glu Leu Met Ala Lys Lys His Ala Ser Tyr Asn Tyr Pro Phe Leu
20 25 30

Glu Pro Val Asp Pro Val Ser Met Asn Leu Pro Thr Tyr Phe Asp Tyr

```
          35                  40                  45

Val Lys Glu Pro Met Asp Leu Gly Thr Ile Ala Lys Lys Leu Asn Asp
     50                  55                  60

Trp Gln Tyr Gln Thr Met Glu Asp Phe Glu Arg Glu Val Arg Leu Val
 65                  70                  75                  80

Phe Lys Asn Cys Tyr Thr Phe Asn Pro Asp Gly Thr Ile Val Asn Met
                 85                  90                  95

Met Gly His Arg Leu Glu Glu Val Phe Asn Ser Lys Trp Ala Asp Arg
            100                 105                 110

Pro
```


<210> 27
<211> 108
<212> PRT
<213> Homo sapiens

<400> 27

```
Met Glu Met Gln Leu Thr Pro Phe Leu Ile Leu Leu Arg Lys Thr Leu
  1               5                  10                  15

Glu Gln Leu Gln Glu Lys Asp Thr Gly Asn Ile Phe Ser Glu Pro Val
            20                  25                  30

Pro Leu Ser Glu Val Pro Asp Tyr Leu Asp His Ile Lys Lys Pro Met
         35                  40                  45

Asp Phe Phe Thr Met Lys Gln Asn Leu Glu Ala Tyr Arg Tyr Leu Asn
     50                  55                  60

Phe Asp Asp Phe Glu Glu Asp Phe Asn Leu Ile Val Ser Asn Cys Leu
 65                  70                  75                  80

Lys Tyr Asn Ala Lys Asp Thr Ile Phe Tyr Arg Ala Ala Val Arg Leu
                 85                  90                  95

Arg Glu Gln Gly Gly Ala Val Val Arg Gln Ala Arg
            100                 105
```

<210> 28
<211> 113

<212> PRT
<213> Homo sapiens

<400> 28
Ser Glu Asp Gln Glu Ala Ile Gln Ala Gln Lys Ile Trp Lys Lys Ala
1 5 10 15

Ile Met Leu Val Trp Arg Ala Ala Ala Asn His Arg Tyr Ala Asn Val
20 25 30

Phe Leu Gln Pro Val Thr Asp Asp Ile Ala Pro Gly Tyr His Ser Ile
35 40 45

Val Gln Arg Pro Met Asp Leu Ser Thr Ile Lys Lys Asn Ile Glu Asn
50 55 60

Gly Leu Ile Arg Ser Thr Ala Glu Phe Gln Arg Asp Ile Met Leu Met
65 70 75 80

Phe Gln Asn Ala Val Met Tyr Asn Ser Ser Asp His Asp Val Tyr His
85 90 95

Met Ala Val Glu Met Gln Arg Asp Val Leu Glu Gln Ile Gln Gln Phe
100 105 110

Leu

<210> 29
<211> 106
<212> PRT
<213> Gallus gallus

<400> 29
Asn Leu Pro Thr Val Asp Pro Ile Ala Val Cys His Glu Leu Tyr Asn
1 5 10 15

Thr Ile Arg Asp Tyr Lys Asp Glu Gln Gly Arg Leu Leu Cys Glu Leu
20 25 30

Phe Ile Arg Ala Pro Lys Arg Arg Asn Gln Pro Asp Tyr Tyr Glu Val
35 40 45

Val Ser Gln Pro Ile Asp Leu Met Lys Ile Gln Gln Lys Leu Lys Met
50 55 60

Glu Glu Tyr Asp Asp Val Asn Val Leu Thr Ala Asp Phe Gln Leu Leu

65 70 75 80

Phe Asn Asn Ala Lys Ala Tyr Tyr Lys Pro Asp Ser Pro Glu Tyr Lys
85 90 95

Ala Ala Cys Lys Leu Trp Glu Leu Tyr Leu
100 105

<210> 30
<211> 112
<212> PRT
<213> Gallus gallus

<400> 30
Ser Ser Pro Gly Tyr Leu Lys Glu Ile Leu Glu Gln Leu Leu Glu Ala
1 5 10 15

Val Ala Val Ala Thr Asn Pro Ser Gly Arg Leu Ile Ser Glu Leu Phe
20 25 30

Gln Lys Leu Pro Ser Lys Val Gln Tyr Pro Asp Tyr Tyr Ala Ile Ile
35 40 45

Lys Glu Pro Ile Asp Leu Lys Thr Ile Ala Gln Arg Ile Gln Asn Gly
50 55 60

Thr Tyr Lys Ser Ile His Ala Met Ala Lys Asp Ile Asp Leu Leu Ala
65 70 75 80

Lys Asn Ala Lys Thr Tyr Asn Glu Pro Gly Ser Gln Val Phe Lys Asp
85 90 95

Ala Asn Ala Ile Lys Lys Ile Phe Asn Met Lys Lys Ala Glu Ile Glu
100 105 110

<210> 31
<211> 112
<212> PRT
<213> Gallus gallus

<400> 31
Thr Ser Phe Met Asp Thr Ser Asn Pro Leu Tyr Gln Leu Tyr Asp Thr
1 5 10 15

Val Arg Ser Cys Arg Asn Asn Gln Gly Gln Leu Ile Ser Glu Pro Phe
20 25 30

Phe Gln Leu Pro Ser Lys Lys Lys Tyr Pro Asp Tyr Tyr Gln Gln Ile
35 40 45

Lys Thr Pro Ile Ser Leu Gln Gln Ile Arg Ala Lys Leu Lys Asn His
50 55 60

Glu Tyr Glu Thr Leu Asp Gln Leu Glu Ala Asp Leu Asn Leu Met Phe
65 70 75 80

Glu Asn Ala Lys Arg Tyr Asn Val Pro Asn Ser Ala Ile Tyr Lys Arg
85 90 95

Val Leu Lys Met Gln Gln Val Met Gln Ala Lys Lys Lys Glu Leu Ala
100 105 110

<210> 32
<211> 113
<212> PRT
<213> Gallus gallus

<400> 32
Ser Lys Lys Asn Met Arg Lys Gln Arg Met Lys Ile Leu Tyr Asn Ala
1 5 10 15

Val Leu Glu Ala Arg Glu Ser Gly Thr Gln Arg Arg Leu Cys Asp Leu
20 25 30

Phe Met Val Lys Pro Ser Lys Lys Asp Tyr Pro Asp Tyr Tyr Lys Ile
35 40 45

Ile Leu Glu Pro Met Asp Leu Lys Met Ile Glu His Asn Ile Arg Asn
50 55 60

Asp Lys Tyr Val Gly Glu Glu Ala Met Ile Asp Asp Met Lys Leu Met
65 70 75 80

Phe Arg Asn Ala Arg His Tyr Asn Glu Glu Gly Ser Gln Val Tyr Asn
85 90 95

Asp Ala His Met Leu Glu Lys Ile Leu Lys Glu Lys Arg Lys Glu Leu

100 105 110

Gly

<210> 33
<211> 115
<212> PRT
<213> Gallus gallus

<400> 33
Lys Lys Ser Lys Tyr Met Thr Pro Met Gln Gln Lys Leu Asn Glu Val
1 5 10 15

Tyr Glu Ala Val Lys Asn Tyr Thr Asp Lys Arg Gly Arg Arg Leu Ser
20 25 30

Ala Ile Phe Leu Arg Leu Pro Ser Arg Ser Glu Leu Pro Asp Tyr Tyr
35 40 45

Ile Thr Ile Lys Lys Pro Val Asp Met Glu Lys Ile Arg Ser His Met
50 55 60

Met Ala Asn Lys Tyr Gln Asp Ile Asp Ser Met Val Glu Asp Phe Val
65 70 75 80

Met Met Phe Asn Asn Ala Cys Thr Tyr Asn Glu Pro Glu Ser Leu Ile
85 90 95

Tyr Lys Asp Ala Leu Val Leu His Lys Val Leu Leu Glu Thr Arg Arg
100 105 110

Glu Ile Glu
115

<210> 34
<211> 112
<212> PRT
<213> Unknown

<220>
<223> Description of Unknown Organism: Cited from
Jeanmougin et al., Trends in Biochemical Sciences,
22:151-153 (1997)

<400> 34

His Asn Ala Pro Phe Asp Lys Thr Lys Phe Asp Glu Val Leu Glu Ala
1 5 10 15

Leu Val Gly Leu Lys Asp Asn Glu Gly Asn Pro Phe Asp Asp Ile Phe
20 25 30

Glu Glu Leu Pro Ser Lys Arg Tyr Phe Pro Asp Tyr Tyr Gln Ile Ile
35 40 45

Gln Lys Pro Ile Cys Tyr Lys Met Met Arg Asn Lys Ala Lys Thr Gly
50 55 60

Lys Tyr Leu Ser Met Gly Asp Phe Tyr Asp Asp Ile Arg Leu Met Val
65 70 75 80

Ser Asn Ala Gln Thr Tyr Asn Met Pro Gly Ser Leu Val Tyr Glu Cys
85 90 95

Ser Val Leu Ile Ala Asn Thr Ala Asn Ser Leu Glu Ser Lys Asp Gly
100 105 110

<210> 35
<211> 113
<212> PRT
<213> Unknown

<220>
<223> Description of Unknown Organism: Cited from Jeanmougin et al., Trends in Biochemical Sciences, 22:151-153 (1997)

<400> 35
Gly Thr Asn Glu Ile Asp Val Pro Lys Val Ile Gln Asn Ile Leu Asp
1 5 10 15

Ala Leu His Glu Glu Lys Asp Glu Gln Gly Arg Phe Leu Ile Asp Ile
20 25 30

Phe Ile Asp Leu Pro Ser Lys Arg Leu Tyr Pro Asp Tyr Tyr Glu Ile
35 40 45

Ile Lys Ser Pro Met Thr Ile Lys Met Leu Glu Lys Arg Phe Lys Lys
50 55 60

```
Gly Glu Tyr Thr Thr Leu Glu Ser Phe Val Lys Asp Leu Asn Gln Met
 65                  70                  75                  80

Phe Ile Asn Ala Lys Thr Tyr Asn Ala Pro Gly Ser Phe Val Tyr Glu
                 85                  90                  95

Asp Ala Glu Lys Leu Ser Gln Leu Ser Ser Ser Leu Ile Ser Ser Phe
            100                 105                 110

Ser
```

<210> 36
<211> 113
<212> PRT
<213> Homo sapiens

<400> 36

```
Gly Thr Asn Glu Ile Asp Val Pro Lys Val Ile Gln Asn Ile Leu Asp
  1               5                  10                  15

Ala Leu His Glu Glu Lys Asp Glu Gln Gly Arg Phe Leu Ile Asp Ile
             20                  25                  30

Phe Ile Asp Leu Pro Ser Lys Arg Leu Tyr Pro Asp Tyr Tyr Glu Ile
         35                  40                  45

Ile Lys Ser Pro Met Thr Ile Lys Met Leu Glu Lys Arg Phe Lys Lys
     50                  55                  60

Gly Glu Tyr Thr Thr Leu Glu Ser Phe Val Lys Asp Leu Asn Gln Met
 65                  70                  75                  80

Phe Ile Asn Ala Lys Thr Tyr Asn Ala Pro Gly Ser Phe Val Tyr Glu
                 85                  90                  95

Asp Ala Glu Lys Leu Ser Gln Leu Ser Ser Ser Leu Ile Ser Ser Phe
            100                 105                 110

Ser
```

<210> 37
<211> 114
<212> PRT
<213> Homo sapiens

<400> 37
Ser Pro Asn Pro Pro Asn Leu Thr Lys Lys Met Lys Lys Ile Val Asp
1 5 10 15

Ala Val Ile Lys Tyr Lys Asp Ser Ser Ser Gly Arg Gln Leu Ser Glu
20 25 30

Val Phe Ile Gln Leu Pro Ser Arg Lys Glu Leu Pro Glu Tyr Tyr Glu
35 40 45

Leu Ile Arg Lys Pro Val Asp Phe Lys Lys Ile Lys Glu Arg Ile Arg
50 55 60

Asn His Lys Tyr Arg Ser Leu Asn Asp Leu Glu Lys Asp Val Met Leu
65 70 75 80

Leu Cys Gln Asn Ala Gln Thr Phe Asn Leu Glu Gly Ser Leu Ile Tyr
85 90 95

Glu Asp Ser Ile Val Leu Gln Ser Val Phe Thr Ser Val Arg Gln Lys
100 105 110

Ile Glu

<210> 38
<211> 113
<212> PRT
<213> Gallus gallus

<400> 38
Ser Pro Asn Pro Pro Lys Leu Thr Lys Gln Met Asn Ala Ile Ile Asp
1 5 10 15

Thr Val Ile Asn Tyr Lys Asp Ser Ser Gly Arg Gln Leu Ser Glu Val
20 25 30

Phe Ile Gln Leu Pro Ser Arg Lys Glu Leu Pro Glu Tyr Tyr Glu Leu
35 40 45

Ile Arg Lys Pro Val Asp Phe Lys Lys Ile Lys Glu Arg Ile Arg Asn
50 55 60

His Lys Tyr Arg Ser Leu Gly Asp Leu Glu Lys Asp Val Met Leu Leu
65 70 75 80

```
Cys His Asn Ala Gln Thr Phe Asn Leu Glu Gly Ser Gln Ile Tyr Glu
                  85                  90                  95

Asp Ser Ile Val Leu Gln Ser Val Phe Lys Ser Ala Arg Gln Lys Ile
            100                 105                 110

Ala
```

<210> 39
<211> 114
<212> PRT
<213> Gallus gallus

<400> 39

```
Ser Pro Asn Pro Pro Asn Leu Thr Lys Lys Met Lys Lys Ile Val Asp
  1               5                  10                  15

Ala Val Ile Lys Tyr Lys Asp Ser Ser Ser Gly Arg Gln Leu Ser Glu
             20                  25                  30

Val Phe Ile Gln Leu Pro Ser Arg Lys Glu Leu Pro Glu Tyr Tyr Glu
          35                  40                  45

Leu Ile Arg Lys Pro Val Asp Phe Lys Lys Ile Lys Glu Arg Ile Arg
     50                  55                  60

Asn His Lys Tyr Arg Ser Leu Asn Asp Leu Glu Lys Asp Val Met Leu
 65                  70                  75                  80

Leu Cys Gln Asn Ala Gln Thr Phe Asn Leu Glu Val Ser Leu Ile Tyr
                  85                  90                  95

Glu Asp Ser Ile Val Leu Gln Ser Val Phe Thr Ser Val Arg Gln Lys
            100                 105                 110

Ile Glu
```

<210> 40
<211> 105
<212> PRT
<213> Homo sapiens

<400> 40

```
Ala Lys Leu Ser Pro Ala Asn Gln Arg Lys Cys Glu Arg Val Leu Leu
```

1 5 10 15

Ala Leu Phe Cys His Glu Pro Cys Arg Pro Leu His Gln Leu Ala Thr
20 25 30

Asp Ser Thr Phe Ser Leu Asp Gln Pro Gly Gly Thr Leu Asp Leu Thr
35 40 45

Leu Ile Arg Ala Arg Leu Gln Glu Lys Leu Ser Pro Pro Tyr Ser Ser
50 55 60

Pro Gln Glu Phe Ala Gln Asp Val Gly Arg Met Phe Lys Gln Phe Asn
65 70 75 80

Lys Leu Thr Glu Asp Lys Ala Asp Val Gln Ser Ile Ile Gly Leu Gln
85 90 95

Arg Phe Phe Glu Thr Arg Met Asn Glu
100 105

<210> 41
<211> 105
<212> PRT
<213> Mus musculus

<400> 41
Ala Lys Leu Ser Pro Ala Asn Gln Arg Lys Cys Glu Arg Val Leu Leu
1 5 10 15

Ala Leu Phe Cys His Glu Pro Cys Arg Pro Leu His Gln Leu Ala Thr
20 25 30

Asp Ser Thr Phe Ser Met Glu Gln Pro Gly Gly Thr Leu Asp Leu Thr
35 40 45

Leu Ile Arg Ala Arg Leu Gln Glu Lys Leu Ser Pro Pro Tyr Ser Ser
50 55 60

Pro Gln Glu Phe Ala Gln Asp Val Gly Arg Met Phe Lys Gln Phe Asn
65 70 75 80

Lys Leu Thr Glu Asp Lys Ala Asp Val Gln Ser Ile Ile Gly Leu Gln
85 90 95

Arg Phe Phe Glu Thr Arg Met Asn Asp
100 105

<210> 42
<211> 108
<212> PRT
<213> Mus sp.

<400> 42
Thr Lys Leu Thr Pro Ile Asp Lys Arg Lys Cys Glu Arg Leu Leu Leu
1 5 10 15

Phe Leu Tyr Cys His Glu Met Ser Leu Ala Phe Gln Asp Pro Val Pro
20 25 30

Leu Thr Val Pro Asp Tyr Tyr Lys Ile Ile Lys Asn Pro Met Asp Leu
35 40 45

Ser Thr Ile Lys Lys Arg Leu Gln Glu Asp Tyr Cys Met Tyr Thr Lys
50 55 60

Pro Glu Asp Phe Val Ala Asp Phe Arg Leu Ile Phe Gln Asn Cys Ala
65 70 75 80

Glu Phe Asn Glu Pro Asp Ser Glu Val Ala Asn Ala Gly Ile Lys Leu
85 90 95

Glu Ser Tyr Phe Glu Glu Leu Leu Lys Asn Leu Tyr
100 105

<210> 43
<211> 13
<212> PRT
<213> Artificial Sequence

<220>
<223> Description of Artificial Sequence: consencus

<220>
<221> VARIANT
<222> (1)
<223> It represents 2 amino acids. They can be any amino acids.

<220>
<221> VARIANT
<222> (3)
<223> It represents 2 to 3 amino acids. They can be any amino acids.

<220>
<221> VARIANT
<222> (5)
<223> It represents 5 to 8 amino acids. They can be any amino acids.

<220>
<221> VARIANT
<222> (7)
<223> It represents one amino acids. It can be any amino acid.

<220>
<221> VARIANT
<222> (10)
<223> It represents 5 amino acids. They can be any amino acids.

<220>
<221> VARIANT
<222> (6)
<223> It represents any amino acid from the group of: P, K, or H.

<220>
<221> VARIANT
<222> (9)
<223> It represents any amino acid from the group of: Y, F, or H.

<220>
<221> VARIANT
<222> (12)
<223> It represents any amino acid from the group of: M, I, or V.

<400> 43
Xaa Phe Xaa Pro Xaa Xaa Xaa Tyr Xaa Xaa Pro Xaa Asp
1 5 10

<210> 44
<211> 20
<212> PRT
<213> Artificial Sequence

<220>

<223> Description of Artificial Sequence: consencus

<400> 44
Trp Pro Phe Met Glu Pro Val Lys Arg Thr Glu Ala Pro Gly Tyr Tyr
1 5 10 15

Glu Val Ile Arg
20